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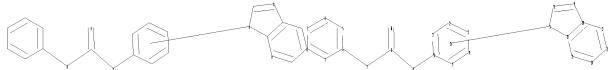
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chain nodes : 7 8 9 16 ring nodes : 1 2 3 4 5 6 10 11 12 13 14 15 17 18 19 20 21 22 23 24 25 chain bonds : 8-9 8-16 9-10 6-7 7-8 ring bonds : $1-2 \quad 1-6 \quad 2-3 \quad 3-4 \quad 4-5 \quad 5-6 \quad 10-11 \quad 10-15 \quad 11-12 \quad 12-13 \quad 13-14 \quad 14-15 \quad 17-18$ 17-21 18-19 19-20 20-21 20-22 21-25 22-23 23-24 24-25 exact/norm bonds : 6-7 7-8 8-9 8-16 9-10 17-18 17-21 18-19 19-20normalized bonds : $1-2 \quad 1-6 \quad 2-3 \quad 3-4 \quad 4-5 \quad 5-6 \quad 10-11 \quad 10-15 \quad 11-12 \quad 12-13 \quad 13-14 \quad 14-15 \quad 20-21$ 20-22 21-25 22-23 23-24 24-25

Match level :

1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:CLASS 8:CLASS 9:CLASS 10:Atom 11:Atom 12:Atom 13:Atom 14:Atom 15:Atom 16:CLASS 17:Atom 18:Atom 19:Atom 20:Atom 21:Atom 22:Atom 23:Atom 24:Atom 25:Atom 26:Atom

L1 STRUCTURE UPLOADED

=> s 11 SAMPLE SEARCH INITIATED 12:14:40 FILE 'REGISTRY' SAMPLE SCREEN SEARCH COMPLETED - 184 TO ITERATE SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS: ONLINE **COMPLETE**

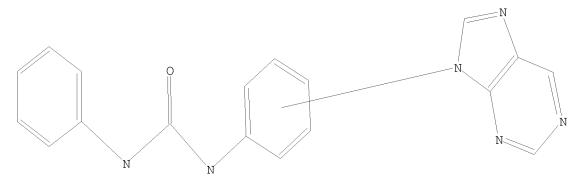
BATCH **COMPLETE**

PROJECTED ITERATIONS: 2867 TO 4493 PROJECTED ANSWERS: 8 TO 329

L2 8 SEA SSS SAM L1

=> d 11

L1 HAS NO ANSWERS
L1 STE



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=> s 11 sss sam

SAMPLE SEARCH INITIATED 12:14:54 FILE 'REGISTRY'

SAMPLE SCREEN SEARCH COMPLETED - 184 TO ITERATE

100.0% PROCESSED 184 ITERATIONS 8 ANSWERS

SEARCH TIME: 00.00.01

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BATCH **COMPLETE**

PROJECTED ITERATIONS: 2867 TO 4493 PROJECTED ANSWERS: 8 TO 329

L3 8 SEA SSS SAM L1

=> s l1 sss full

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FULL SCREEN SEARCH COMPLETED - 3577 TO ITERATE

100.0% PROCESSED 3577 ITERATIONS 269 ANSWERS

SEARCH TIME: 00.00.01

L4 269 SEA SSS FUL L1

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FILE COVERS 1907 - 6 Oct 2009 VOL 151 ISS 15

FILE LAST UPDATED: 5 Oct 2009 (20091005/ED)

REVISED CLASS FIELDS (/NCL) LAST RELOADED: Aug 2009

USPTO MANUAL OF CLASSIFICATIONS THESAURUS ISSUE DATE: Aug 2009

CAplus now includes complete International Patent Classification (IPC) reclassification data for the third quarter of 2009.

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=> s 14 L5 9 L4

=> d ibib abs hitstr 1-9

L5 ANSWER 1 OF 9 CAPLUS COPYRIGHT 2009 ACS on STN

ACCESSION NUMBER: 2006:1090595 CAPLUS

DOCUMENT NUMBER: 145:438456

TITLE: Preparation of purine derivatives as receptor-tyrosine

kinase activity inhibitors

INVENTOR(S): Hoelzemann, Guenter; Crassier, Helene; Rautenberg,

Wilfried; Jonczyk, Alfred Merck Patent GmbH, Germany

SOURCE: PCT Int. Appl., 92pp.

CODEN: PIXXD2

DOCUMENT TYPE: Patent LANGUAGE: German

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT ASSIGNEE(S):

PATENT NO. KIND				D	DATE		APPLICATION NO.					DATE					
WO 2006108482			A1	_	20061019		WO 2006-EP2380					20060315					
	W:	ΑE,	AG,	AL,	AM,	ΑT,	ΑU,	AZ,	BA,	BB,	BG,	BR,	BW,	BY,	BZ,	CA,	CH,
		CN,	CO,	CR,	CU,	CZ,	DE,	DK,	DM,	DZ,	EC,	EE,	EG,	ES,	FI,	GB,	GD,
		GE,	GH,	GM,	HR,	HU,	ID,	IL,	IN,	IS,	JP,	ΚE,	KG,	KM,	KN,	KP,	KR,
		KΖ,	LC,	LK,	LR,	LS,	LT,	LU,	LV,	LY,	MA,	MD,	MG,	MK,	MN,	MW,	MX,
		MΖ,	NA,	NG,	NI,	NO,	NΖ,	OM,	PG,	PH,	PL,	PT,	RO,	RU,	SC,	SD,	SE,
		SG,	SK,	SL,	SM,	SY,	ТJ,	TM,	TN,	TR,	TT,	TZ,	UA,	UG,	US,	UZ,	VC,
		VN,	YU,	ZA,	ZM,	ZW											
	RW:	ΑT,	BE,	BG,	CH,	CY,	CZ,	DE,	DK,	EE,	ES,	FI,	FR,	GB,	GR,	HU,	ΙE,
		IS,	ΙT,	LT,	LU,	LV,	MC,	NL,	PL,	PT,	RO,	SE,	SI,	SK,	TR,	BF,	ВJ,
		CF,	CG,	CI,	CM,	GA,	GN,	GO,	GW,	ML,	MR,	NE,	SN,	TD,	TG,	BW.	GH,

GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM DE 102005017259 20061019 DE 2005-102005017259 20050414 Α1 AU 2006233530 20061019 AU 2006-233530 20060315 A1 CA 2604294 20061019 CA 2006-2604294 20060315 Α1 EP 1869047 A1 20071226 EP 2006-723450 20060315 AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IS, IT, LI, LT, LU, LV, MC, NL, PL, PT, RO, SE, SI, SK, TR JP 2008535874 Τ 20080904 JP 2008-505752 20060315 US 20080214582 Α1 20080904 US 2008-910776 20080418 PRIORITY APPLN. INFO.: DE 2005-102005017259A 20050414 WO 2006-EP2380 W 20060315

OTHER SOURCE(S): CASREACT 145:438456

GΙ

or

AB The invention relates to compds. I [R1 = H, A; R2, R3 = H, A, Hal, OH, OA, CN; R4 = Ar, Het1; R5, R6 = H, A; X = OH, NH2; A = C1-10-alkyl, optionally substituted with 1 to 7 F or Cl; Ar = (un)substituted Ph optionally substituted with 1 to 3 from the following, Hal, A, OA, OH, C2-6-alkenyl, C2-6-alkynyl, NO2, NR5R6, C(:O)NR5R6, CO2H, CO2A, CN, CHO, COA, Ph, (CH2)nHet, O(CH2)nHet, NH(CH2)nHet, O(CH2)nCyc, N(CH2)nCyc, O(CH2)mNR5R6, NR1(CH2)mNR5R6, O(CH2)mNR5R6; Het = (un)saturated or aromatic, mono-

bicyclic heterocycle containing 1 to 4 N, O and S and optionally substituted with 1 to 3 Hal, A, OA, Ph, CO2A, CN, CC(:O); Het1 = mono- or bicyclic, aromatic heterocycle containing 1 to 4 N, O and S and optionally substituted with

1 to 3 Hal, A, OA, OH, C2-6-alkenyl, C2-6-alkynyl, NO2, NR5R6, C(:0)NR5R6, CO2H, CO2A, CN, CHO, COA, Ph, (CH2)nHet, O(CH2)nHet, NH(CH2)nHet, O(CH2)nCyc, N(CH2)nCyc, O(CH2)mNR5R6, NR1(CH2)mNR5R6, O(CH2)mNR1O(CH2)mNR5R6; Cyc = C3-7-cycloalkyl; Hal = F, Cl, Br, I; n = 0, 1, 2, 3, 4; m = 1, 2, 3, 4] or their pharmaceutically acceptable salts, solvates, tautomers, stereoisomers or their mixts., which are inhibitors of tyrosine kinases, in particular TIE-2, and the Raf-kinases and can be also be used for treating tumors. The procedure for the preparation of I comprises: carbamoylation of purinylanilines II with (a) isocyanates, R4NCO; or (b) carbamoylation by sequential addition of chloroformates

followed by amines R4NH2; or, (c) by solvolysis or hydrogenolysis of protected derivs. of II and its salts. Thus, 1-[4-(6-aminopurin-9-y1)pheny1]-3-[3-(trifluoromethy1)pheny1]urea [I; R1 =R2 = R3 = H; R4 = C6H4CF3-3; X = NH2] was prepd, from 9-(4-aminophenyl) adenine [II; R1 = R2 = R3 = H; X = NH2] via carbamoylation with 3-CF2C6H4NCO in CH2Cl2 containing Et3N. The enzyme inhibiting activity of I [R1 = R2 = R3 = H; R4 = C6H4CF3-3; X = NH2] was determined [IC50 = 14 nmol/L vs. Tyrosine kinase receptor Tie-2 and IC50 = 3.6]nmol/L vs. Vascular endothelial growth factor receptors (VEGFR)]. 912539-35-6P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(preparation and N-deprotection of; preparation of purine derivs. as receptor-tyrosine kinase activity inhibitors)

RN 912539-35-6 CAPLUS

ΙT

CN 1-Pyrrolidinecarboxylic acid, 3-[2-[[[[4-(6-amino-9H-purin-9yl)phenyl]amino]carbonyl]amino]-4-(trifluoromethyl)phenoxy]-, 1,1-dimethylethyl ester (CA INDEX NAME)

(preparation of purine derivs. as receptor-tyrosine kinase activity inhibitors)

912539-16-3 CAPLUS RN

Urea, N-[4-(6-amino-9H-purin-9-y1)pheny1]-N'-[2-(3-pyrrolidinyloxy)-5-CN (trifluoromethyl)phenyl]- (CA INDEX NAME)

RN 912539-17-4 CAPLUS

CN Urea, N-[4-(6-amino-9H-purin-9-yl)phenyl]-N'-[3-(trifluoromethyl)phenyl]- (CA INDEX NAME)

RN 912539-18-5 CAPLUS

CN Urea, N-[4-(1,6-dihydro-6-oxo-9H-purin-9-yl)phenyl]-N'-[3-(trifluoromethyl)phenyl]- (CA INDEX NAME)

RN 912539-19-6 CAPLUS

CN Urea, N-[4-(6-amino-9H-purin-9-yl)phenyl]-N'-[2-fluoro-5-(trifluoromethyl)phenyl]- (CA INDEX NAME)

RN 912539-20-9 CAPLUS

CN Urea, N-[4-(6-amino-9H-purin-9-yl)phenyl]-N'-[3-(trifluoromethoxy)phenyl]- (CA INDEX NAME)

RN 912539-22-1 CAPLUS

CN Urea, N-[4-(1,6-dihydro-6-oxo-9H-purin-9-yl)phenyl]-N'-[2-fluoro-5-(trifluoromethyl)phenyl]- (CA INDEX NAME)

RN 912539-23-2 CAPLUS

CN Urea, N-[4-(6-amino-9H-purin-9-yl)phenyl]-N'-[4-(1H-1,2,4-triazol-1-yl)-3-(trifluoromethyl)phenyl]- (CA INDEX NAME)

RN 912539-24-3 CAPLUS

CN Urea, N-[4-(6-amino-9H-purin-9-yl)phenyl]-N'-[2-(1H-1,2,4-triazol-1-yl)-5-(trifluoromethyl)phenyl]- (CA INDEX NAME)

RN 912539-25-4 CAPLUS

CN Urea, N-[4-(6-amino-9H-purin-9-yl)phenyl]-N'-[2-(1H-1,2,3-triazol-1-yl)-5-(trifluoromethyl)phenyl]- (CA INDEX NAME)

RN 912539-26-5 CAPLUS

CN Urea, N-[4-(6-amino-9H-purin-9-y1)pheny1]-N'-[4-(3-pyrrolidinyloxy)-3-(trifluoromethyl)phenyl]- (CA INDEX NAME)

RN 912539-27-6 CAPLUS

CN Urea, N-[4-(6-amino-8-methyl-9H-purin-9-yl)phenyl]-N'-[3-(trifluoromethyl)phenyl]- (CA INDEX NAME)

RN 912539-29-8 CAPLUS

CN Urea, N-[4-(6-amino-9H-purin-9-yl)phenyl]-N'-[3-(1-methylethyl)phenyl]- (CA INDEX NAME)

RN 912539-40-3 CAPLUS

CN Urea, N-[4-(6-amino-9H-purin-9-yl)phenyl]-N'-[2-fluoro-5-(trifluoromethyl)phenyl]-, 2,2,2-trifluoroacetate (1:1) (CA INDEX NAME)

CM 1

CRN 912539-19-6

CMF C19 H13 F4 N7 O

CM 2

CRN 76-05-1 CMF C2 H F3 O2

RN 912539-41-4 CAPLUS

CN Urea, N-[4-(6-amino-9H-purin-9-yl)phenyl]-N'-[3-(trifluoromethoxy)phenyl]-, 2,2,2-trifluoroacetate (1:1) (CA INDEX NAME)

CM 1

CRN 912539-20-9 CMF C19 H14 F3 N7 O2

CM 2

CRN 76-05-1 CMF C2 H F3 O2

RN 912539-43-6 CAPLUS

CN Urea, N-[4-(6-amino-9H-purin-9-yl)phenyl]-N'-[4-(1H-1,2,4-triazol-1-yl)-3-(trifluoromethyl)phenyl]-, 2,2,2-trifluoroacetate (1:1) (CA INDEX NAME)

CM 1

CRN 912539-23-2 CMF C21 H15 F3 N10 O

CM 2

CRN 76-05-1 CMF C2 H F3 O2

RN 912539-44-7 CAPLUS

CN Urea, N-[4-(6-amino-9H-purin-9-yl)phenyl]-N'-[2-(1H-1,2,4-triazol-1-yl)-5-(trifluoromethyl)phenyl]-, 2,2,2-trifluoroacetate (1:1) (CA INDEX NAME)

CM 1

CRN 912539-24-3 CMF C21 H15 F3 N10 O

CM 2

CRN 76-05-1 CMF C2 H F3 O2

RN 912539-45-8 CAPLUS

CN Urea, N-[4-(6-amino-9H-purin-9-yl)phenyl]-N'-[2-(1H-1,2,3-triazol-1-yl)-5-(trifluoromethyl)phenyl]-, 2,2,2-trifluoroacetate (1:1) (CA INDEX NAME)

CM 1

CRN 912539-25-4

CMF C21 H15 F3 N10 O

CM 2

CRN 76-05-1 CMF C2 H F3 O2

RN 912539-46-9 CAPLUS

CN Urea, N-[4-(6-amino-9H-purin-9-yl)phenyl]-N'-[4-(3-pyrrolidinyloxy)-3-(trifluoromethyl)phenyl]-, hydrochloride (1:2) (CA INDEX NAME)

●2 HC1

RN 912539-48-1 CAPLUS

CN Urea, N-[4-(6-amino-9H-purin-9-yl)phenyl]-N'-[3-[5-(1,1-dimethylethyl)-3-isoxazolyl]phenyl]-, 2,2,2-trifluoroacetate (1:1) (CA INDEX NAME)

CM 1

CRN 912539-47-0 CMF C25 H24 N8 O2

CM 2

CRN 76-05-1 CMF C2 H F3 O2

IT 912539-36-7P 912539-37-8P

RL: SPN (Synthetic preparation); PREP (Preparation)

(preparation of purine derivs. as receptor-tyrosine kinase activity inhibitors)

RN 912539-36-7 CAPLUS

CN Urea, N-[4-(6-amino-9H-purin-9-y1)pheny1]-N'-[2-(3-pyrrolidinyloxy)-5-(trifluoromethyl)phenyl]-, hydrochloride (1:2) (CA INDEX NAME)

●2 HC1

RN 912539-37-8 CAPLUS

CN Urea, N-[4-(6-amino-9H-purin-9-y1)pheny1]-N'-[3-(trifluoromethy1)pheny1]-, 2,2,2-trifluoroacetate (1:1) (CA INDEX NAME)

CM 1

CRN 912539-17-4 CMF C19 H14 F3 N7 O

CM 2

CRN 76-05-1 CMF C2 H F3 O2

REFERENCE COUNT: 4 THERE ARE 4 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L5 ANSWER 2 OF 9 CAPLUS COPYRIGHT 2009 ACS on STN

ACCESSION NUMBER: 2005:962206 CAPLUS

DOCUMENT NUMBER: 143:266944

TITLE: Preparation of heteroarylphenylurea derivatives as Raf

inhibitors

INVENTOR(S): Oikawa, Nobuhiro; Mizuguchi, Eisaku; Morikami, Kenji;

Shimma, Nobuo; Ishii, Nobuya; Tsukaguchi, Toshiyuki;

Ozawa, Sawako

PATENT ASSIGNEE(S): Chugai Seiyaku Kabushiki Kaisha, Japan

SOURCE: PCT Int. Appl., 296 pp.

CODEN: PIXXD2

DOCUMENT TYPE: Patent LANGUAGE: Japanese

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PA'	PATENT NO.				KIND DATE				APPLICATION NO.					DATE			
WO	WO 2005080330			A1	20050901			WO 2005-JP2923					20050223				
	W:	ΑE,	AG,	AL,	ΑM,	ΑT,	ΑU,	AZ,	ΒA,	BB,	BG,	BR,	BW,	BY,	BZ,	CA,	CH,
		CN,	CO,	CR,	CU,	CZ,	DE,	DK,	DM,	DZ,	EC,	EE,	EG,	ES,	FΙ,	GB,	GD,
		GE,	GH,	GM,	HR,	HU,	ID,	IL,	IN,	IS,	JP,	ΚE,	KG,	KP,	KR,	KΖ,	LC,
		LK,	LR,	LS,	LT,	LU,	LV,	MA,	MD,	MG,	MK,	MN,	MW,	MX,	MZ,	NA,	NI,
		NO,	NZ,	OM,	PG,	PH,	PL,	PT,	RO,	RU,	SC,	SD,	SE,	SG,	SK,	SL,	SY,
		ΤJ,	TM,	TN,	TR,	TT,	TZ,	UA,	UG,	US,	UZ,	VC,	VN,	YU,	ZA,	ZM,	ZW
	RW:	BW,	GH,	GM,	KE,	LS,	MW,	MZ,	NA,	SD,	SL,	SZ,	TZ,	UG,	ZM,	ZW,	AM,
		AZ,	BY,	KG,	KΖ,	MD,	RU,	ТJ,	TM,	AT,	BE,	BG,	CH,	CY,	CZ,	DE,	DK,
		EE,	ES,	FI,	FR,	GB,	GR,	HU,	ΙE,	IS,	IT,	LT,	LU,	MC,	NL,	PL,	PT,
		RO,	SE,	SI,	SK,	TR,	BF,	ВJ,	CF,	CG,	CI,	CM,	GA,	GN,	GQ,	GW,	ML,
		MR,	NE,	SN,	TD,	TG	·	·	·		•	•	•	•		·	·
EP	EP 1724258			A1 20061122				EP 2005-719431					20050223				
	R:	AT,	BE,	BG,	CH,	CY,	CZ,	DE,	DK,	EE,	ES,	FI,	FR,	GB,	GR,	HU,	IE,
								NL,							TR	•	·
US	US 20080119466				A1				US 2006-590026					·			
	RIORITY APPLN. INFO.:								JP 2004-47037 JP 2004-248856				Ž	A 20040223			

OTHER SOURCE(S): MARPAT 143:266944

GT

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

Title compds. I [R1, R2, R5 = H, halo, etc.; R3, R4 = H, halo, etc.; R6, R7 = H, halo; Z1, Z2 = H, OH, etc.; Q = II; G1 = C-Y2, N; ring A =benzene, etc.; Y1, Y2 = H, halo, etc.] were prepared For example, treatment of 1-[4-(6-aminopurin-9-yl)phenyl]-3-[4-chloro-3-(trifluoromethyl)phenyl]urea hydrochloride, e.g., prepared from adenine in 5 steps, with propylisocyanate afforded compound III. In Raf-1 enzyme inhibition assays, the IC50 value of compound III was 0.013 μM . Cpmpounds I are claimed useful for the treatment of cancer, diabetes, etc. 863673-42-1P ΙT 863673-35-2P 863673-36-3P 863673-54-5P 863673-58-9P 863673-68-1P 863674-28-6P 863674-35-5P 863674-36-6P 863674-48-0P 863674-50-4P 863674-56-0P 863674-57-1P 863674-58-2P 863675-11-0P

863675-12-1P RL: PAC (Pharmacological activity); RCT (Reactant); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); RACT (Reactant or reagent); USES (Uses)

(preparation of heteroarylphenylurea derivs. as Raf inhibitors for treatment of cancer and diabetes)

863673-35-2 CAPLUS RN

CN Imidodicarbonic acid, 2-[9-[4-[[[[4-chloro-3-(trifluoromethyl)phenyl]amino]carbonyl]amino]phenyl]-9H-purin-6-yl]-, 1,3-bis(1,1-dimethylethyl) ester (CA INDEX NAME)

863673-36-3 CAPLUS RN

Urea, N-[4-(6-amino-9H-purin-9-yl)phenyl]-N'-[4-chloro-3-CN (trifluoromethyl)phenyl]-, hydrochloride (1:1) (CA INDEX NAME)

RN 863673-42-1 CAPLUS

CN Urea, N-[4-chloro-3-(trifluoromethyl)phenyl]-N'-[4-[6-(methylamino)-9H-purin-9-yl]phenyl]-, hydrochloride (1:1) (CA INDEX NAME)

● HCl

RN 863673-54-5 CAPLUS

CN Imidodicarbonic acid, 2-[9-[4-[[[[4-chloro-3-(trifluoromethyl)phenyl]amino]carbonyl]hydroxyamino]phenyl]-9H-purin-6-yl]-, 1,3-bis(1,1-dimethylethyl) ester (CA INDEX NAME)

RN 863673-58-9 CAPLUS

CN Urea, N-[4-(6-chloro-9H-purin-9-yl)phenyl]-N'-[4-chloro-3-(trifluoromethyl)phenyl]-N-hydroxy- (CA INDEX NAME)

RN 863673-68-1 CAPLUS

CN Imidodicarbonic acid, 2-[9-[4-[[[[4-chloro-3-(trifluoromethyl)phenyl]hydroxyamino]carbonyl]amino]phenyl]-9H-purin-6-yl]-, 1,3-bis(1,1-dimethylethyl) ester (CA INDEX NAME)

RN 863674-28-6 CAPLUS

CN Urea, N-[9-[4-[[[[4-chloro-3-(trifluoromethyl)phenyl]amino]carbonyl]amino]phenyl]-9H-purin-6-yl]-N'-2-propen-1-yl- (CA INDEX NAME)

RN 863674-35-5 CAPLUS

CN Urea, N-[4-(6-amino-8-iodo-9H-purin-9-yl)phenyl]-N'-[4-chloro-3-(trifluoromethyl)phenyl]- (CA INDEX NAME)

RN 863674-36-6 CAPLUS

CN Urea, N-[4-(6-amino-8-ethenyl-9H-purin-9-yl)phenyl]-N'-[4-chloro-3-(trifluoromethyl)phenyl]- (CA INDEX NAME)

RN 863674-48-0 CAPLUS

CN Urea, N-[4-[6-(methylamino)-9H-purin-9-yl]phenyl]-N'-[3-(trifluoromethyl)phenyl]- (CA INDEX NAME)

RN 863674-50-4 CAPLUS

CN Urea, N-[4-chloro-3-(trifluoromethyl)phenyl]-N'-[4-[8-iodo-6-(methylamino)-9H-purin-9-yl]phenyl]- (CA INDEX NAME)

RN 863674-56-0 CAPLUS

CN Urea, N-[4-(6-amino-9H-purin-9-yl)phenyl]-N'-[3-[(4-methyl-1-piperazinyl)methyl]-5-(trifluoromethyl)phenyl]- (CA INDEX NAME)

RN 863674-57-1 CAPLUS

CN Urea, N-[4-(6-amino-8-iodo-9H-purin-9-yl)phenyl]-N'-[3-[(4-methyl-1-piperazinyl)methyl]-5-(trifluoromethyl)phenyl]- (CA INDEX NAME)

RN 863674-58-2 CAPLUS

CN Urea, N-[4-(6-amino-8-ethenyl-9H-purin-9-yl)phenyl]-N'-[3-[(4-methyl-1-piperazinyl)methyl]-5-(trifluoromethyl)phenyl]- (CA INDEX NAME)

RN 863675-11-0 CAPLUS

CN 9H-Purine-6-carboxylic acid, 9-[4-[[[[4-chloro-3-(trifluoromethyl)phenyl]amino]carbonyl]amino]phenyl]-, methyl ester (CA INDEX NAME)

RN 863675-12-1 CAPLUS

CN 9H-Purine-6-carboxylic acid, 9-[4-[[[[4-chloro-3-(trifluoromethyl)phenyl]amino]carbonyl]amino]phenyl]- (CA INDEX NAME)

ΙT	863673-11-4P	863673-37-4P	863673-38-5P
	863673-39-6P	863673-40-9P	863673-41-0P
	863673-53-4P	863673-55-6P	863673-56-7P
	863673-59-0P	863673-60-3P	863673-61-4P

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863673-69-2P
                 863673-63-6P
863673-62-5P
                                   863674-01-5P
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863675-58-5P
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU
(Therapeutic use); BIOL (Biological study); PREP (Preparation); USES
(Uses)
   (preparation of heteroarylphenylurea derivs. as Raf inhibitors for treatment
   of cancer and diabetes)
863673-11-4 CAPLUS
Urea, N-[4-chloro-3-(trifluoromethyl)phenyl]-N'-[4-(9H-purin-9-yl)phenyl]-
  (CA INDEX NAME)
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RN

CN

RN 863673-37-4 CAPLUS

CN Urea, N-[4-(6-amino-9H-purin-9-yl)phenyl]-N'-[3,5-bis(trifluoromethyl)phenyl]-, hydrochloride (1:1) (CA INDEX NAME)

● HCl

RN 863673-38-5 CAPLUS

CN Urea, N-[4-(6-amino-9H-purin-9-yl)phenyl]-N'-[2-chloro-5-(trifluoromethyl)phenyl]-, hydrochloride (1:1) (CA INDEX NAME)

● HCl

RN 863673-39-6 CAPLUS

CN Urea, N-[4-(6-amino-9H-purin-9-yl)-2-fluorophenyl]-N'-[4-chloro-3-(trifluoromethyl)phenyl]-, hydrochloride (1:1) (CA INDEX NAME)

RN 863673-40-9 CAPLUS

CN Urea, N-[4-(2-amino-9H-purin-9-yl)phenyl]-N'-[4-chloro-3-(trifluoromethyl)phenyl]-, hydrochloride (1:1) (CA INDEX NAME)

● HCl

RN 863673-41-0 CAPLUS

CN Urea, N-[4-chloro-3-(trifluoromethyl)phenyl]-N'-[4-[6-[(2-methoxyethyl)amino]-9H-purin-9-yl]phenyl]-, hydrochloride (1:1) (CA INDEX NAME)

● HCl

RN 863673-53-4 CAPLUS

CN Urea, N'-[4-chloro-3-(trifluoromethyl)phenyl]-N-hydroxy-N-[4-(9H-purin-9-yl)phenyl]- (CA INDEX NAME)

RN 863673-55-6 CAPLUS

CN Urea, N-[4-(6-amino-9H-purin-9-yl)phenyl]-N'-[4-chloro-3-(trifluoromethyl)phenyl]-N-hydroxy-, hydrochloride (1:1) (CA INDEX NAME)

● HCl

RN 863673-56-7 CAPLUS

CN Urea, N'-[4-chloro-3-(trifluoromethyl)phenyl]-N-hydroxy-N-[4-(6-methyl-9H-purin-9-yl)phenyl]- (CA INDEX NAME)

RN 863673-59-0 CAPLUS

CN Urea, N'-[4-chloro-3-(trifluoromethyl)phenyl]-N-hydroxy-N-[4-[6-(methylamino)-9H-purin-9-yl]phenyl]- (CA INDEX NAME)

RN 863673-60-3 CAPLUS

CN Urea, N'-[4-chloro-3-(trifluoromethyl)phenyl]-N-hydroxy-N-[4-[6-[methyl(phenylmethyl)amino]-9H-purin-9-yl]phenyl]- (CA INDEX NAME)

RN 863673-61-4 CAPLUS

CN Urea, N'-[4-chloro-3-(trifluoromethyl)phenyl]-N-hydroxy-N-[4-[6-(4-morpholinyl)-9H-purin-9-yl]phenyl]- (CA INDEX NAME)

RN 863673-62-5 CAPLUS

CN Urea, N'-[4-chloro-3-(trifluoromethyl)phenyl]-N-[4-[6-(dimethylamino)-9H-purin-9-yl]phenyl]-N-hydroxy- (CA INDEX NAME)

RN 863673-63-6 CAPLUS

CN Urea, N'-[4-chloro-3-(trifluoromethyl)phenyl]-N-hydroxy-N-[4-[6-[(2-hydroxyethyl)methylamino]-9H-purin-9-yl]phenyl]- (CA INDEX NAME)

RN 863673-69-2 CAPLUS

CN Urea, N'-[4-(6-amino-9H-purin-9-yl)phenyl]-N-[4-chloro-3-(trifluoromethyl)phenyl]-N-hydroxy-, hydrochloride (1:1) (CA INDEX NAME)

RN 863673-72-7 CAPLUS

CN Urea, N-[4-chloro-3-(trifluoromethyl)phenyl]-N-hydroxy-N'-[4-(6-methyl-9H-purin-9-yl)phenyl]- (CA INDEX NAME)

RN 863673-74-9 CAPLUS

CN Urea, N-[4-chloro-3-(trifluoromethyl)phenyl]-N'-[4-[6-(dimethylamino)-9H-purin-9-yl]phenyl]-N-hydroxy- (CA INDEX NAME)

RN 863674-01-5 CAPLUS

CN Methanimidamide, N'-[9-[4-[[[[4-chloro-3-(trifluoromethyl)phenyl]amino]carbonyl]amino]phenyl]-9H-purin-6-yl]-N,N-dimethyl-, hydrochloride (1:1) (CA INDEX NAME)

● HCl

CN Pentanamide, 2-amino-N-[9-[4-[[[[4-chloro-3-(trifluoromethyl)phenyl]amino]carbonyl]amino]phenyl]-9H-purin-6-yl]-4-methyl-, hydrochloride (1:1), (2S)- (CA INDEX NAME)

Absolute stereochemistry.

● HCl

RN 863674-03-7 CAPLUS

CN Acetamide, 2-amino-N-[9-[4-[[[[4-chloro-3-(trifluoromethyl)phenyl]amino]carbonyl]amino]phenyl]-9H-purin-6-yl]-, hydrochloride (1:1) (CA INDEX NAME)

● HCl

RN 863674-04-8 CAPLUS

CN Acetamide, N-[9-[4-[[[4-chloro-3-(trifluoromethyl)phenyl]amino]carbonyl]amino]phenyl]-9H-purin-6-yl]-2-(methylamino)-, hydrochloride (1:1) (CA INDEX NAME)

RN 863674-05-9 CAPLUS

CN 2-Pyrrolidinecarboxamide, N-[9-[4-[[[[4-chloro-3-(trifluoromethyl)phenyl]amino]carbonyl]amino]phenyl]-9H-purin-6-yl]-, hydrochloride (1:1), (2S)- (CA INDEX NAME)

Absolute stereochemistry.

● HCl

RN 863674-06-0 CAPLUS

CN Propanamide, 2-amino-N-[9-[4-[[[[4-chloro-3-(trifluoromethyl)phenyl]amino]carbonyl]amino]phenyl]-9H-purin-6-yl]-, hydrochloride (1:1), (2S)- (CA INDEX NAME)

RN

863674-07-1 CAPLUS Butanamide, 2-amino-N-[9-[4-[[[[4-chloro-3-CN (trifluoromethyl)phenyl]amino]carbonyl]amino]phenyl]-9H-purin-6-yl]-3,3dimethyl-, hydrochloride (1:1), (2S)- (CA INDEX NAME)

Absolute stereochemistry.

● HCl

RN 863674-08-2 CAPLUS

Butanamide, 2-amino-N-[9-[4-[[[[4-chloro-3-CN (trifluoromethyl)phenyl]amino]carbonyl]amino]phenyl]-9H-purin-6-yl]-3methyl-, hydrochloride (1:1), (2R)- (CA INDEX NAME)

RN 863674-09-3 CAPLUS

CN Pentanoic acid, 4-amino-5-[[9-[4-[[[[4-chloro-3-(trifluoromethyl)phenyl]amino]carbonyl]amino]phenyl]-9H-purin-6-yl]amino]-5-oxo-, hydrochloride (1:1), (4S)- (CA INDEX NAME)

Absolute stereochemistry.

● HCl

RN 863674-10-6 CAPLUS

CN L-Glutamine, N-[9-[4-[[[[4-chloro-3-(trifluoromethyl)phenyl]amino]carbonyl]amino]phenyl]-9H-purin-6-yl]-, monohydrochloride (9CI) (CA INDEX NAME)

RN 863674-11-7 CAPLUS

CN Hexanamide, 2,6-diamino-N-[9-[4-[[[[4-chloro-3-(trifluoromethyl)phenyl]amino]carbonyl]amino]phenyl]-9H-purin-6-yl]-, hydrochloride (1:2), (2S)- (CA INDEX NAME)

Absolute stereochemistry.

●2 HC1

RN 863674-12-8 CAPLUS

CN Pentanamide, N-[9-[4-[[[[4-chloro-3-(trifluoromethyl)phenyl]amino]carbonyl]amino]phenyl]-9H-purin-6-yl]-4-methyl-2-(methylamino)-, hydrochloride (1:1), (2S)- (CA INDEX NAME)

RN

863674-13-9 CAPLUS Pentanamide, N-[9-[4-[[[[4-chloro-3-CN (trifluoromethyl)phenyl]amino]carbonyl]amino]phenyl]-9H-purin-6-yl]- (CA INDEX NAME)

863674-14-0 CAPLUS RN

Propanamide, N-[9-[4-[[[[4-chloro-3-CN (trifluoromethyl)phenyl]amino]carbonyl]amino]phenyl]-9H-purin-6-yl]-2,2dimethyl- (CA INDEX NAME)

863674-15-1 CAPLUS RN

CN Acetamide, N-[9-[4-[[[4-chloro-3-(trifluoromethyl)phenyl]amino]carbonyl]amino]phenyl]-9H-purin-6-yl]-2-[2-1]-(2-methoxyethoxy)ethoxy]- (CA INDEX NAME)

PAGE 1-B

RN 863674-16-2 CAPLUS

CN Methanesulfonamide, N-[9-[4-[[[[4-chloro-3-(trifluoromethyl)phenyl]amino]carbonyl]amino]phenyl]-9H-purin-6-yl]-N-(methylsulfonyl)- (CA INDEX NAME)

RN 863674-17-3 CAPLUS

CN Hexanamide, N-[9-[4-[[[[4-chloro-3-(trifluoromethyl)phenyl]amino]carbonyl]amino]phenyl]-9H-purin-6-yl]- (CA INDEX NAME)

RN 863674-18-4 CAPLUS

CN Carbamic acid, [9-[4-[[[[4-chloro-3-(trifluoromethyl)phenyl]amino]carbonyl]amino]phenyl]-9H-purin-6-yl]-, ethyl ester (9CI) (CA INDEX NAME)

RN 863674-19-5 CAPLUS

CN Carbamic acid, [9-[4-[[[[4-chloro-3-(trifluoromethyl)phenyl]amino]carbonyl]amino]phenyl]-9H-purin-6-yl]-, 2-methylpropyl ester (9CI) (CA INDEX NAME)

RN 863674-20-8 CAPLUS

CN Carbamic acid, [9-[4-[[[[4-chloro-3-(trifluoromethyl)phenyl]amino]carbonyl]amino]phenyl]-9H-purin-6-yl]-, 2-propenyl ester (9CI) (CA INDEX NAME)

$$H_2C = CH - CH_2 - O - C - NH$$

$$NH - C - NH$$

$$NH - C - NH$$

RN 863674-21-9 CAPLUS

CN Carbamic acid, [9-[4-[[[[4-chloro-3-(trifluoromethyl)phenyl]amino]carbonyl]amino]phenyl]-9H-purin-6-yl]-, 2-methoxyethyl ester (9CI) (CA INDEX NAME)

RN 863674-22-0 CAPLUS

CN Urea, N-[4-chloro-3-(trifluoromethyl)phenyl]-N'-[4-[6-(2-oxo-3-vert)]

oxazolidinyl)-9H-purin-9-yl]phenyl]- (CA INDEX NAME)

RN 863674-23-1 CAPLUS

CN Carbamic acid, [9-[4-[[[[4-chloro-3-(trifluoromethyl)phenyl]amino]carbonyl]amino]phenyl]-9H-purin-6-yl]-, 2-(methylamino)ethyl ester, monohydrochloride (9CI) (CA INDEX NAME)

● HCl

RN 863674-24-2 CAPLUS

CN Carbamic acid, [9-[4-[[[4-chloro-3-(trifluoromethyl)phenyl]amino]carbonyl]amino]phenyl]-9H-purin-6-yl]-, 2-aminoethyl ester, monohydrochloride (9CI) (CA INDEX NAME)

$$H_2N-CH_2-CH_2-O-C-NH$$
 $NH-C-NH$ CF_3 $C1$

● HCl

RN 863674-25-3 CAPLUS

CN Urea, N-[9-[4-[[[4-chloro-3-(trifluoromethyl)phenyl]amino]carbonyl]amino]phenyl]-9H-purin-6-yl]-N'-propyl-(CA INDEX NAME)

RN 863674-26-4 CAPLUS

CN Urea, N-[9-[4-[[[[4-chloro-3-(trifluoromethyl)phenyl]amino]carbonyl]amino]phenyl]-9H-purin-6-yl]-N'-cyclohexyl- (CA INDEX NAME)

RN 863674-27-5 CAPLUS

CN Urea, N-[9-[4-[[[4-chloro-3-(trifluoromethyl)phenyl]amino]carbonyl]amino]phenyl]-9H-purin-6-yl]-N'-ethyl- (CA INDEX NAME)

RN 863674-29-7 CAPLUS

CN Urea, N-[9-[4-[[[[4-chloro-3-(trifluoromethy1)pheny1]amino]carbony1]amino]pheny1]-9H-purin-6-y1]-N-methyl-N'-propyl- (CA INDEX NAME)

RN 863674-30-0 CAPLUS

CN Urea, N-[9-[4-[[[[4-chloro-3-(trifluoromethyl)phenyl]amino]carbonyl]amino]phenyl]-9H-purin-6-yl]-N'-(2-hydroxyethyl)- (CA INDEX NAME)

RN 863674-31-1 CAPLUS

CN Urea, N-[4-chloro-3-(trifluoromethyl)phenyl]-N'-[4-[6-[(2-hydroxyethyl)methylamino]-9H-purin-9-yl]phenyl]- (CA INDEX NAME)

RN 863674-32-2 CAPLUS

CN Urea, N-[4-chloro-3-(trifluoromethyl)phenyl]-N'-[4-[6-(4-morpholinyl)-9H-purin-9-yl]phenyl]- (CA INDEX NAME)

RN 863674-33-3 CAPLUS

CN Urea, N-[4-chloro-3-(trifluoromethyl)phenyl]-N'-[4-[6-(pentylamino)-9H-purin-9-yl]phenyl]- (CA INDEX NAME)

RN 863674-34-4 CAPLUS

CN Urea, N-[4-chloro-3-(trifluoromethyl)phenyl]-N'-[4-[6-(1-piperazinyl)-9H-purin-9-yl]phenyl]-, hydrochloride (1:1) (CA INDEX NAME)

● HCl

RN 863674-37-7 CAPLUS

CN Urea, N-[4-[6-amino-8-(1,2-dihydroxyethyl)-9H-purin-9-yl]phenyl]-N'-[4-chloro-3-(trifluoromethyl)phenyl]- (CA INDEX NAME)

RN 863674-38-8 CAPLUS

CN Urea, N-[4-[6-amino-8-(hydroxymethyl)-9H-purin-9-yl]phenyl]-N'-[4-chloro-3-(trifluoromethyl)phenyl]- (CA INDEX NAME)

RN 863674-39-9 CAPLUS

CN Urea, N-[4-chloro-3-(trifluoromethyl)phenyl]-N'-[4-[6-[[2-(4-morpholinyl)ethyl]amino]-9H-purin-9-yl]phenyl]- (CA INDEX NAME)

RN 863674-40-2 CAPLUS

CN Urea, N-[4-[6-amino-8-[(dimethylamino)methyl]-9H-purin-9-yl]phenyl]-N'-[4-chloro-3-(trifluoromethyl)phenyl]- (CA INDEX NAME)

RN 863674-41-3 CAPLUS

CN

Urea, N-[9-[4-[[[[4-chloro-3(trifluoromethyl)phenyl]amino]carbonyl]amino]phenyl]-8-ethenyl-9H-purin-6yl]-N'-propyl- (CA INDEX NAME)

RN 863674-42-4 CAPLUS

CN Urea, N-[4-(6-amino-8-methoxy-9H-purin-9-yl)phenyl]-N'-[4-chloro-3-(trifluoromethyl)phenyl]- (CA INDEX NAME)

RN 863674-43-5 CAPLUS

CN Urea, N-[9-[4-[[[4-chloro-3-(trifluoromethyl)phenyl]amino]carbonyl]amino]phenyl]-8-(1,2-dihydroxyethyl)-9H-purin-6-yl]-N'-propyl- (CA INDEX NAME)

RN 863674-44-6 CAPLUS

CN Urea, N-[4-(6-amino-9H-purin-9-yl)-2-bromophenyl]-N'-[4-chloro-3-(trifluoromethyl)phenyl]- (CA INDEX NAME)

RN 863674-45-7 CAPLUS

CN Urea, N-[4-(6-amino-9H-purin-9-yl)phenyl]-N'-[4-bromo-3-(trifluoromethyl)phenyl]-, hydrochloride (1:1) (CA INDEX NAME)

● HCl

RN 863674-46-8 CAPLUS

CN Urea, N-[4-[6-amino-8-(2-methoxyethoxy)-9H-purin-9-yl]phenyl]-N'-[4-chloro-3-(trifluoromethyl)phenyl]- (CA INDEX NAME)

RN 863674-51-5 CAPLUS

CN Urea, N-[4-chloro-3-(trifluoromethyl)phenyl]-N'-[4-[8-methoxy-6-(methylamino)-9H-purin-9-yl]phenyl]- (CA INDEX NAME)

RN 863674-52-6 CAPLUS

CN Urea, N-[4-chloro-3-(trifluoromethyl)phenyl]-N'-[4-[8-ethoxy-6-(methylamino)-9H-purin-9-yl]phenyl]- (CA INDEX NAME)

RN 863674-53-7 CAPLUS

 $\label{eq:cn_sol} \text{CN} \qquad \text{Urea, N-[4-chloro-3-(trifluoromethyl)phenyl]-N'-[4-[8-(2-methoxyethoxy)-6-methoxyethoxy]-0. } \\ \text{Urea, N-[4-chloro-3-(trifluoromethyl)phenyl]-N'-[4-[8-(4-methoxyethoxyethoxy]-0. } \\ \text{Urea, N-[4-chloro-3-(trifluoromethyl)phenyl]-N'-[4-[8-(4-methoxyethoxyethoxy]-0. } \\ \text{Urea, N-[4-chloro-3-(trifluoromethyl)phenyl]-N'-[4-[8-(4-methoxyethoxyethoxyethoxy]-0. } \\ \text{Urea, N-[4-chloro-3-(trifluoromethyl)phenyl]-N'-[4-[8-(4-methoxyethoxyethoxyethoxyethoxyethoxyethoxy]-0. } \\ \text{Urea, N-[4-chloro-3-(trifluoromethyl)phenyl]-N'-[4-[8-(4-methoxyeth$

(methylamino)-9H-purin-9-yl]phenyl]- (CA INDEX NAME)

RN 863674-54-8 CAPLUS

CN Urea, N-[4-chloro-3-(trifluoromethyl)phenyl]-N'-[4-[8-[2-(dimethylamino)ethoxy]-6-(methylamino)-9H-purin-9-yl]phenyl]- (CA INDEX NAME)

RN 863674-55-9 CAPLUS

CN Urea, N-[4-[6-(methylamino)-9H-purin-9-yl]phenyl]-N'-[3-[(4-methyl-1-piperazinyl)methyl]-5-(trifluoromethyl)phenyl]- (CA INDEX NAME)

RN 863674-59-3 CAPLUS

CN Urea, N-[4-(6-amino-9H-purin-9-yl)phenyl]-N'-[3-[(dimethylamino)methyl]-5-(trifluoromethyl)phenyl]- (CA INDEX NAME)

RN 863674-60-6 CAPLUS

CN Urea, N-[3-[(dimethylamino)methyl]-5-(trifluoromethyl)phenyl]-N'-[4-[6-(methylamino)-9H-purin-9-yl]phenyl]- (CA INDEX NAME)

RN 863674-65-1 CAPLUS

CN Urea, N-[4-[6-(methylamino)-9H-purin-9-yl]phenyl]-N'-[4-(4-methyl-1-piperazinyl)-3-(trifluoromethyl)phenyl]- (CA INDEX NAME)

RN 863674-66-2 CAPLUS

CN Urea, N-[4-(6-amino-9H-purin-9-yl)phenyl]-N'-[4-[[2-(dimethylamino)ethyl]methylamino]-3-(trifluoromethyl)phenyl]- (CA INDEX NAME)

RN 863674-67-3 CAPLUS

CN Urea, N-[4-(6-amino-9H-purin-9-yl)phenyl]-N'-[4-(dimethylamino)-3-(trifluoromethyl)phenyl]- (CA INDEX NAME)

RN 863674-68-4 CAPLUS

CN Urea, N-[4-(6-amino-9H-purin-9-y1)pheny1]-N'-[3-[(4-methyl-1-

piperazinyl)carbonyl]-5-(trifluoromethyl)phenyl]- (CA INDEX NAME)

RN 863674-69-5 CAPLUS

CN Benzamide, 3-[[[[4-(6-amino-9H-purin-9-yl)phenyl]amino]carbonyl]amino]-N-[2-(dimethylamino)ethyl]-5-(trifluoromethyl)- (CA INDEX NAME)

RN 863674-70-8 CAPLUS

CN Urea, N-[4-[6-(methylamino)-9H-purin-9-yl]phenyl]-N'-[3-[(4-methyl-1-piperazinyl)carbonyl]-5-(trifluoromethyl)phenyl]- (CA INDEX NAME)

RN 863674-71-9 CAPLUS

CN Benzamide, N-[2-(dimethylamino)ethyl]-3-[[[[4-[6-(methylamino)-9H-purin-9-yl]phenyl]amino]carbonyl]amino]-5-(trifluoromethyl)- (CA INDEX NAME)

RN 863674-72-0 CAPLUS

CN Urea, N-[4-(6-amino-9H-purin-9-y1)pheny1]-N'-[4-(4-methyl-1-piperazinyl)-3-(trifluoromethyl)phenyl]- (CA INDEX NAME)

RN 863674-73-1 CAPLUS

CN Urea, N-[4-(dimethylamino)-3-(trifluoromethyl)phenyl]-N'-[4-[6-(methylamino)-9H-purin-9-yl]phenyl]- (CA INDEX NAME)

RN 863674-74-2 CAPLUS

CN Urea, N-[4-(6-amino-9H-purin-9-yl)phenyl]-N'-[3-bromo-5-(trifluoromethyl)phenyl]- (CA INDEX NAME)

RN 863674-75-3 CAPLUS

CN Urea, N-[4-(1,2-dihydroxyethyl)-3-(trifluoromethyl)phenyl]-N'-[4-[6-(methylamino)-9H-purin-9-yl]phenyl]- (CA INDEX NAME)

RN 863674-76-4 CAPLUS

CN Urea, N-[4-(hydroxymethyl)-3-(trifluoromethyl)phenyl]-N'-[4-[6-(methylamino)-9H-purin-9-yl]phenyl]- (CA INDEX NAME)

RN 863674-77-5 CAPLUS

CN Urea, N-[4-[6-(methylamino)-9H-purin-9-yl]phenyl]-N'-[4-[(4-methyl-1-piperazinyl)methyl]-3-(trifluoromethyl)phenyl]- (CA INDEX NAME)

RN 863674-78-6 CAPLUS

CN Urea, N-[4-[6-(methylamino)-9H-purin-9-yl]phenyl]-N'-[4-(4-morpholinylmethyl)-3-(trifluoromethyl)phenyl]- (CA INDEX NAME)

RN 863674-79-7 CAPLUS

CN Urea, N-[3-(dimethylamino)-5-(trifluoromethyl)phenyl]-N'-[4-[6-(methylamino)-9H-purin-9-yl]phenyl]- (CA INDEX NAME)

RN 863674-80-0 CAPLUS

CN Urea, N-[4-(6-amino-9H-purin-9-yl)phenyl]-N'-[4-[2-(dimethylamino)ethoxy]-3-(trifluoromethyl)phenyl]- (CA INDEX NAME)

RN 863674-81-1 CAPLUS

CN Urea, N-[4-(6-amino-9H-purin-9-yl)phenyl]-N'-[4-[2-(4-morpholinyl)ethoxy]-3-(trifluoromethyl)phenyl]- (CA INDEX NAME)

RN 863674-82-2 CAPLUS

CN Urea, N-[3-amino-5-(trifluoromethyl)phenyl]-N'-[4-[6-(methylamino)-9H-purin-9-yl]phenyl]- (CA INDEX NAME)

RN 863674-83-3 CAPLUS

CN Urea, N-[4-[2-(dimethylamino)ethoxy]-3-(trifluoromethyl)phenyl]-N'-[4-[6-(methylamino)-9H-purin-9-yl]phenyl]- (CA INDEX NAME)

RN 863674-84-4 CAPLUS

CN Urea, N-[4-[6-(methylamino)-9H-purin-9-yl]phenyl]-N'-[4-[2-(4-morpholinyl)ethoxy]-3-(trifluoromethyl)phenyl]- (CA INDEX NAME)

RN 863674-85-5 CAPLUS

CN Benzamide, N-[2-hydroxy-1-(hydroxymethyl)ethyl]-3-[[[[4-[6-(methylamino)-9H-purin-9-yl]phenyl]amino]carbonyl]amino]-5-(trifluoromethyl)- (CA INDEX NAME)

RN 863674-86-6 CAPLUS

CN Benzamide, 3-[[[[4-(6-amino-9H-purin-9-yl)phenyl]amino]carbonyl]amino]-N-[3-hydroxy-2-(hydroxymethyl)propyl]-5-(trifluoromethyl)- (CA INDEX NAME)

RN 863674-87-7 CAPLUS

CN Benzamide, 3-[[[[4-(6-amino-9H-purin-9-yl)phenyl]amino]carbonyl]amino]-N-[2-hydroxy-1-(hydroxymethyl)ethyl]-5-(trifluoromethyl)- (CA INDEX NAME)

RN 863674-88-8 CAPLUS

CN Benzamide, N-[3-hydroxy-2-(hydroxymethyl)propyl]-3-[[[[4-[6-(methylamino)-9H-purin-9-yl]phenyl]amino]carbonyl]amino]-5-(trifluoromethyl)- (CA INDEX NAME)

RN 863674-89-9 CAPLUS

CN Benzamide, 3-[[[[4-[6-(methylamino)-9H-purin-9-yl]phenyl]amino]carbonyl]amino]-N-[2-(4-morpholinyl)ethyl]-5-(trifluoromethyl)- (CA INDEX NAME)

RN 863674-90-2 CAPLUS

CN Urea, N-[4-[(dimethylamino)methyl]-3-(trifluoromethyl)phenyl]-N'-[4-[6-(methylamino)-9H-purin-9-yl]phenyl]- (CA INDEX NAME)

RN 863674-91-3 CAPLUS

CN Urea, N-[4-[[[2-(dimethylamino)ethyl]amino]methyl]-3- (trifluoromethyl)phenyl]-N'-[4-[6-(methylamino)-9H-purin-9-yl]phenyl]- (CA INDEX NAME)

RN 863674-92-4 CAPLUS

CN Urea, N-[4-(6-amino-9H-purin-9-yl)phenyl]-N'-[4-[(1-methyl-4-piperidinyl)oxy]-3-(trifluoromethyl)phenyl]- (CA INDEX NAME)

RN 863674-93-5 CAPLUS

CN Urea, N-[4-[6-(methylamino)-9H-purin-9-yl]phenyl]-N'-[4-[(1-methyl-4-piperidinyl)oxy]-3-(trifluoromethyl)phenyl]- (CA INDEX NAME)

RN 863674-94-6 CAPLUS

CN Urea, N-[4-[2-(dimethylamino)ethyl]-3-(trifluoromethyl)phenyl]-N'-[4-[6-(methylamino)-9H-purin-9-yl]phenyl]- (CA INDEX NAME)

RN 863674-95-7 CAPLUS

CN Urea, N-[4-[6-(methylamino)-9H-purin-9-yl]phenyl]-N'-[4-[2-(4-methyl-1-piperazinyl)ethyl]-3-(trifluoromethyl)phenyl]- (CA INDEX NAME)

RN 863674-96-8 CAPLUS

CN Urea, N-[4-[6-(methylamino)-9H-purin-9-y1]pheny1]-N'-[4-[2-(4-morpholiny1)ethy1]-3-(trifluoromethy1)pheny1]- (CA INDEX NAME)

RN 863674-97-9 CAPLUS

CN Urea, N-[3-[2-(dimethylamino)ethyl]-5-(trifluoromethyl)phenyl]-N'-[4-[6-(methylamino)-9H-purin-9-yl]phenyl]- (CA INDEX NAME)

RN 863674-98-0 CAPLUS

CN Urea, N-[4-[6-(methylamino)-9H-purin-9-yl]phenyl]-N'-[3-[2-(4-methyl-1-piperazinyl)ethyl]-5-(trifluoromethyl)phenyl]- (CA INDEX NAME)

RN 863674-99-1 CAPLUS

CN Urea, N-[4-[6-(methylamino)-9H-purin-9-yl]phenyl]-N'-[3-[2-(4-morpholinyl)ethyl]-5-(trifluoromethyl)phenyl]- (CA INDEX NAME)

RN 863675-00-7 CAPLUS

CN Urea, N-[4-[3-(dimethylamino)propyl]-3-(trifluoromethyl)phenyl]-N'-[4-[6-(methylamino)-9H-purin-9-yl]phenyl]- (CA INDEX NAME)

RN 863675-01-8 CAPLUS

CN Urea, N-[4-[6-(methylamino)-9H-purin-9-yl]phenyl]-N'-[4-[3-(4-methyl-1-piperazinyl)propyl]-3-(trifluoromethyl)phenyl]- (CA INDEX NAME)

RN 863675-02-9 CAPLUS

CN Urea, N-[4-[6-(methylamino)-9H-purin-9-yl]phenyl]-N'-[4-[3-(4-morpholinyl)propyl]-3-(trifluoromethyl)phenyl]- (CA INDEX NAME)

RN 863675-03-0 CAPLUS

CN Urea, N-[4-[6-(methylamino)-9H-purin-9-yl]phenyl]-N'-[4-[3-(1-pyrrolidinyl)propyl]-3-(trifluoromethyl)phenyl]- (CA INDEX NAME)

RN 863675-04-1 CAPLUS

CN Urea, N-[4-[6-(methylamino)-9H-purin-9-yl]phenyl]-N'-[4-[3-(1-piperidinyl)propyl]-3-(trifluoromethyl)phenyl]- (CA INDEX NAME)

RN 863675-05-2 CAPLUS

CN Urea, N-[3-[2-(dimethylamino)ethoxy]-5-(trifluoromethyl)phenyl]-N'-[4-[6-(methylamino)-9H-purin-9-yl]phenyl]- (CA INDEX NAME)

RN 863675-06-3 CAPLUS

CN Urea, N-[4-[6-(methylamino)-9H-purin-9-yl]phenyl]-N'-[3-[(1-methyl-4-piperidinyl)oxy]-5-(trifluoromethyl)phenyl]- (CA INDEX NAME)

RN 863675-13-2 CAPLUS

CN 9H-Purine-6-carboxamide, 9-[4-[[[[4-chloro-3-(trifluoromethyl)phenyl]amino]carbonyl]amino]phenyl]-N-methyl- (CA INDEX NAME)

RN 863675-17-6 CAPLUS

CN Benzamide, 3-[[[4-(6-amino-9H-purin-9-y1)pheny1]amino]carbony1]amino]-N-[2-(4-morpholiny1)ethy1]-5-(trifluoromethy1)- (CA INDEX NAME)

RN 863675-18-7 CAPLUS

CN Urea, N-[4-[6-(methylamino)-9H-purin-9-yl]phenyl]-N'-[4-(1-piperazinylmethyl)-3-(trifluoromethyl)phenyl]- (CA INDEX NAME)

RN 863675-19-8 CAPLUS

CN Urea, N-[4-[6-(methylamino)-9H-purin-9-yl]phenyl]-N'-[4-(1-pyrrolidinylmethyl)-3-(trifluoromethyl)phenyl]- (CA INDEX NAME)

RN 863675-20-1 CAPLUS

CN Urea, N-[4-[(4-ethyl-1-piperazinyl)methyl]-3-(trifluoromethyl)phenyl]-N'-[4-[6-(methylamino)-9H-purin-9-yl]phenyl]- (CA INDEX NAME)

RN 863675-21-2 CAPLUS

CN Urea, N-[4-[6-(methylamino)-9H-purin-9-yl]phenyl]-N'-[4-[[[2-(1-pyrrolidinyl)ethyl]amino]methyl]-3-(trifluoromethyl)phenyl]- (CA INDEX NAME)

RN 863675-22-3 CAPLUS

CN Urea, N-[4-[6-(methylamino)-9H-purin-9-yl]phenyl]-N'-[4-(1-piperidinylmethyl)-3-(trifluoromethyl)phenyl]- (CA INDEX NAME)

RN 863675-23-4 CAPLUS

CN Urea, N-[4-(cyclohexylmethyl)-3-(trifluoromethyl)phenyl]-N'-[4-[6-(methylamino)-9H-purin-9-yl]phenyl]- (CA INDEX NAME)

RN 863675-25-6 CAPLUS

CN Urea, N-[4-[6-(methylamino)-9H-purin-9-yl]phenyl]-N'-[4-[[(tetrahydro-2H-pyran-4-yl)amino]methyl]-3-(trifluoromethyl)phenyl]- (CA INDEX NAME)

RN 863675-26-7 CAPLUS

CN Urea, N-[4-[[[3-(dimethylamino)propyl]amino]methyl]-3- (trifluoromethyl)phenyl]-N'-[4-[6-(methylamino)-9H-purin-9-yl]phenyl]- (CA INDEX NAME)

RN 863675-27-8 CAPLUS

CN Urea, N-[4-[6-(methylamino)-9H-purin-9-yl]phenyl]-N'-[4-[[[3-(4-morpholinyl)propyl]amino]methyl]-3-(trifluoromethyl)phenyl]- (CA INDEX NAME)

RN 863675-28-9 CAPLUS

CN Urea, N-[4-[6-(methylamino)-9H-purin-9-yl]phenyl]-N'-[4-[(4-piperidinylamino)methyl]-3-(trifluoromethyl)phenyl]- (CA INDEX NAME)

RN 863675-29-0 CAPLUS

CN Urea, N-[4-[6-(methylamino)-9H-purin-9-yl]phenyl]-N'-[4-[[(4-piperidinylmethyl)amino]methyl]-3-(trifluoromethyl)phenyl]- (CA INDEX NAME)

RN 863675-30-3 CAPLUS

CN Urea, N-[4-[(cyclohexylmethylamino)methyl]-3-(trifluoromethyl)phenyl]-N'-[4-[6-(methylamino)-9H-purin-9-yl]phenyl]- (CA INDEX NAME)

RN 863675-31-4 CAPLUS

CN Urea, N-[4-[(4-amino-1-piperidinyl)methyl]-3-(trifluoromethyl)phenyl]-N'[4-[6-(methylamino)-9H-purin-9-yl]phenyl]- (CA INDEX NAME)

RN 863675-32-5 CAPLUS

CN Urea, N-[4-[(4-hydroxy-1-piperidinyl)methyl]-3-(trifluoromethyl)phenyl]-N'-[4-[6-(methylamino)-9H-purin-9-yl]phenyl]- (CA INDEX NAME)

RN 863675-33-6 CAPLUS

CN Urea, N-[4-[[[2-(dimethylamino)ethyl]methylamino]methyl]-3-(trifluoromethyl)phenyl]-N'-[4-[6-(methylamino)-9H-purin-9-yl]phenyl]-(CA INDEX NAME)

RN 863675-34-7 CAPLUS

CN Urea, N-[4-[6-(methylamino)-9H-purin-9-yl]phenyl]-N'-[4-[[4-(1-methylethyl)-1-piperazinyl]methyl]-3-(trifluoromethyl)phenyl]- (CA INDEX NAME)

RN 863675-35-8 CAPLUS

CN Urea, N-[4-[[[3-(dimethylamino)propyl]methylamino]methyl]-3- (trifluoromethyl)phenyl]-N'-[4-[6-(methylamino)-9H-purin-9-yl]phenyl]- (CA INDEX NAME)

RN 863675-36-9 CAPLUS

CN Urea, N-[4-[6-(methylamino)-9H-purin-9-yl]phenyl]-N'-[3-[2-(1-piperidinyl)ethyl]-5-(trifluoromethyl)phenyl]- (CA INDEX NAME)

RN 863675-37-0 CAPLUS

CN Urea, N-[4-[6-(methylamino)-9H-purin-9-yl]phenyl]-N'-[3-[2-(1-pyrrolidinyl)ethyl]-5-(trifluoromethyl)phenyl]- (CA INDEX NAME)

RN 863675-38-1 CAPLUS

CN Urea, N-[4-[3-(dimethylamino)propoxy]-3-(trifluoromethyl)phenyl]-N'-[4-[6-(methylamino)-9H-purin-9-yl]phenyl]- (CA INDEX NAME)

RN 863675-39-2 CAPLUS

CN Urea, N-[4-[6-(methylamino)-9H-purin-9-yl]phenyl]-N'-[4-[2-(1-piperidinyl)ethyl]-3-(trifluoromethyl)phenyl]- (CA INDEX NAME)

RN 863675-40-5 CAPLUS

CN Urea, N-[4-[6-(methylamino)-9H-purin-9-yl]phenyl]-N'-[4-[2-(1-pyrrolidinyl)ethyl]-3-(trifluoromethyl)phenyl]- (CA INDEX NAME)

RN 863675-41-6 CAPLUS

CN Urea, N-[4-[2-(cyclohexylmethylamino)ethyl]-3-(trifluoromethyl)phenyl]-N'-[4-[6-(methylamino)-9H-purin-9-yl]phenyl]- (CA INDEX NAME)

RN 863675-42-7 CAPLUS

CN Urea, N-[4-[2-[[2-(dimethylamino)ethyl]methylamino]ethyl]-3-(trifluoromethyl)phenyl]-N'-[4-[6-(methylamino)-9H-purin-9-yl]phenyl]-(CA INDEX NAME)

RN 863675-43-8 CAPLUS

CN Urea, N-[4-[6-(methylamino)-9H-purin-9-yl]phenyl]-N'-[4-[2-[4-(1-methylethyl)-1-piperazinyl]ethyl]-3-(trifluoromethyl)phenyl]- (CA INDEX NAME)

RN 863675-44-9 CAPLUS

CN Urea, N-[4-[2-[[3-(dimethylamino)propyl]methylamino]ethyl]-3- (trifluoromethyl)phenyl]-N'-[4-[6-(methylamino)-9H-purin-9-yl]phenyl]- (CA INDEX NAME)

RN 863675-45-0 CAPLUS

CN Urea, N-[4-[2-(4-ethyl-1-piperazinyl)ethyl]-3-(trifluoromethyl)phenyl]-N'[4-[6-(methylamino)-9H-purin-9-yl]phenyl]- (CA INDEX NAME)

RN 863675-46-1 CAPLUS

CN Urea, N-[4-[6-(methylamino)-9H-purin-9-yl]phenyl]-N'-[4-[2-(1-piperazinyl)ethyl]-3-(trifluoromethyl)phenyl]- (CA INDEX NAME)

RN 863675-47-2 CAPLUS

CN Urea, N-[4-(2-methoxyethoxy)-3-(trifluoromethyl)phenyl]-N'-[4-[6-(methylamino)-9H-purin-9-yl]phenyl]- (CA INDEX NAME)

RN 863675-48-3 CAPLUS

CN Urea, N-[4-[2-(2-methoxyethoxy)ethoxy]-3-(trifluoromethyl)phenyl]-N'-[4-[6-(methylamino)-9H-purin-9-yl]phenyl]- (CA INDEX NAME)

RN 863675-49-4 CAPLUS

CN Urea, N-[4-[6-(methylamino)-9H-purin-9-y1]pheny1]-N'-[4-[2-(4-piperidiny1)ethoxy]-3-(trifluoromethy1)pheny1]- (CA INDEX NAME)

RN 863675-50-7 CAPLUS

CN Urea, N-[4-[6-(methylamino)-9H-purin-9-yl]phenyl]-N'-[4-(4-piperidinylmethoxy)-3-(trifluoromethyl)phenyl]- (CA INDEX NAME)

RN 863675-51-8 CAPLUS

CN Urea, N-[4-[6-(methylamino)-9H-purin-9-yl]phenyl]-N'-[3-[3-(1-pyrrolidinyl)propyl]-5-(trifluoromethyl)phenyl]- (CA INDEX NAME)

RN 863675-52-9 CAPLUS

CN Urea, N-[4-[(3,5-dimethyl-1-piperazinyl)methyl]-3-(trifluoromethyl)phenyl]-N'-[4-[6-(methylamino)-9H-purin-9-yl]phenyl]- (CA INDEX NAME)

RN 863675-53-0 CAPLUS

CN Urea, N-[4-[6-(methylamino)-9H-purin-9-yl]phenyl]-N'-[4-[2-(4-pyridinyl)ethyl]-3-(trifluoromethyl)phenyl]- (CA INDEX NAME)

RN 863675-54-1 CAPLUS

CN Urea, N-[4-[6-(methylamino)-9H-purin-9-yl]phenyl]-N'-[3-[3-(4-morpholinyl)propyl]-5-(trifluoromethyl)phenyl]- (CA INDEX NAME)

RN 863675-55-2 CAPLUS

CN Urea, N-[4-[6-(methylamino)-9H-purin-9-yl]phenyl]-N'-[4-[[4-(1-oxopentyl)-1-piperazinyl]methyl]-3-(trifluoromethyl)phenyl]- (CA INDEX NAME)

RN 863675-56-3 CAPLUS

CN Urea, N-[4-[(4-acetyl-1-piperazinyl)methyl]-3-(trifluoromethyl)phenyl]-N'-[4-[6-(methylamino)-9H-purin-9-yl]phenyl]- (CA INDEX NAME)

RN 863675-57-4 CAPLUS

CN Urea, N-[4-[[4-(2,2-dimethyl-1-oxopropyl)-1-piperazinyl]methyl]-3-(trifluoromethyl)phenyl]-N'-[4-[6-(methylamino)-9H-purin-9-yl]phenyl]-(CA INDEX NAME)

RN 863675-58-5 CAPLUS

CN Urea, N-[4-[6-(methylamino)-9H-purin-9-yl]phenyl]-N'-[4-(4-pyridinylmethyl)-3-(trifluoromethyl)phenyl]- (CA INDEX NAME)

RN 863675-59-6 CAPLUS

CN Benzenepropanamide, N-methyl-4-[[[[4-[6-(methylamino)-9H-purin-9-yl]phenyl]amino]carbonyl]amino]-2-(trifluoromethyl)- (CA INDEX NAME)

863675-83-6P 863675-90-5P 863675-93-8P 863675-94-9P 863675-95-0P 863675-96-1P 863675-97-2P 863676-01-1P 863676-02-2P 863676-03-3P 863676-06-6P 863676-07-7P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(preparation of heteroarylphenylurea derivs. as Raf inhibitors for treatment of cancer and diabetes)

RN 863675-80-3 CAPLUS

CN Carbamic acid, [(1S)-1-[[[9-[4-[[[[4-chloro-3-(trifluoromethyl)phenyl]amino]carbonyl]amino]phenyl]-9H-purin-6-yl]amino]carbonyl]-3-methylbutyl]-, 1,1-dimethylethyl ester (9CI) (CIINDEX NAME)

Absolute stereochemistry.

RN 863675-81-4 CAPLUS

CN Carbamic acid, [2-[[[[9-[4-[[[[4-chloro-3-(trifluoromethyl)phenyl]amino]carbonyl]amino]phenyl]-9H-purin-6-yl]amino]carbonyl]oxy]ethyl]methyl-, 1,1-dimethylethyl ester (9CI) (CA

INDEX NAME)

RN 863675-82-5 CAPLUS

CN Urea, N-[4-(6-amino-8-formyl-9H-purin-9-yl)phenyl]-N'-[4-chloro-3-(trifluoromethyl)phenyl]- (CA INDEX NAME)

RN 863675-83-6 CAPLUS

CN Imidodicarbonic acid, 2-[9-[4-[[[[4-bromo-3-(trifluoromethyl)phenyl]amino]carbonyl]amino]phenyl]-9H-purin-6-yl]-, 1,3-bis(1,1-dimethylethyl) ester (CA INDEX NAME)

RN 863675-90-5 CAPLUS

CN Carbamic acid, methyl[9-[4-[[[[4-(4-methyl-1-piperazinyl)-3-(trifluoromethyl)phenyl]amino]carbonyl]amino]phenyl]-9H-purin-6-yl]-, 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)

RN 863675-93-8 CAPLUS

CN Carbamic acid, [9-[4-[[[[4-bromo-3-(trifluoromethyl)phenyl]amino]carbonyl]amino]phenyl]-9H-purin-6-yl]methyl-, 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)

RN 863675-94-9 CAPLUS

CN Carbamic acid, [9-[4-[[[[4-ethenyl-3-(trifluoromethyl)phenyl]amino]carbonyl]amino]phenyl]-9H-purin-6-yl]methyl-, 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)

RN 863675-95-0 CAPLUS

CN Carbamic acid, [9-[4-[[[[4-(1,2-dihydroxyethyl)-3-(trifluoromethyl)phenyl]amino]carbonyl]amino]phenyl]-9H-purin-6-yl]methyl-, 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)

RN 863675-96-1 CAPLUS

CN Carbamic acid, [9-[4-[[[[4-formyl-3-(trifluoromethyl)phenyl]amino]carbonyl]amino]phenyl]-9H-purin-6-yl]methyl-, 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)

RN 863675-97-2 CAPLUS

CN Carbamic acid, [9-[4-[[[[4-(hydroxymethyl)-3-(trifluoromethyl)phenyl]amino]carbonyl]amino]phenyl]-9H-purin-6-yl]methyl-, 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)

RN 863676-01-1 CAPLUS

CN Benzoic acid, 3-[[[[4-[6-[[(1,1-dimethylethoxy)carbonyl]methylamino]-9H-purin-9-yl]phenyl]amino]carbonyl]amino]-5-(trifluoromethyl)-, phenylmethyl ester (CA INDEX NAME)

RN 863676-02-2 CAPLUS

CN Benzoic acid, 3-[[[[4-[6-[[(1,1-dimethylethoxy)carbonyl]methylamino]-9H-purin-9-yl]phenyl]amino]carbonyl]amino]-5-(trifluoromethyl)- (CA INDEX NAME)

RN 863676-03-3 CAPLUS

CN Carbamic acid, [9-[4-[[[3-[[[2-hydroxy-1-(hydroxymethyl)ethyl]amino]carbonyl]-5-(trifluoromethyl)phenyl]amino]carbonyl]amino]phenyl]-9H-purin-6-yl]methyl-, 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)

RN 863676-06-6 CAPLUS

CN Carbamic acid, [9-[4-[[[4-(2-hydroxyethy1)-3-(trifluoromethy1)pheny1]amino]carbony1]amino]pheny1]-9H-purin-6-y1]methy1-, 1,1-dimethy1ethy1 ester (9CI) (CA INDEX NAME)

RN 863676-07-7 CAPLUS

CN Carbamic acid, methyl[9-[4-[[[[4-(2-oxoethyl)-3-(trifluoromethyl)phenyl]amino]carbonyl]amino]phenyl]-9H-purin-6-yl]-, 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)

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REFERENCE COUNT: 36 THERE ARE 36 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

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ACCESSION NUMBER: 2003:319714 CAPLUS

DOCUMENT NUMBER: 138:338157

TITLE: Preparation of 1,4-disubstituted benzo-fused ureas as

cytokine inhibitors

INVENTOR(S): Cirillo, Pier F.; Hammach, Abdelhakim; Regan, John R.

PATENT ASSIGNEE(S): Boehringer Ingelheim Pharmaceuticals, Inc., USA

SOURCE: PCT Int. Appl., 100 pp.

CODEN: PIXXD2

DOCUMENT TYPE: Patent LANGUAGE: English

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

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                      KIND DATE
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PRIORITY APPLN. INFO.:
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                                         WO 2002-US32809 W 20021011
OTHER SOURCE(S): MARPAT 138:338157
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* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

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AB The title compds. [I; ring A = fused (un)saturated ring containing 3-5 carbon atoms (wherein ring A or the Ph ring to which it is fused is optionally substituted); G = (un)substituted 5-membered heteroaryl; Q = (un)substituted naphthyl, benzocyclobutanyl, indanyl, etc.; X = 0, S] which are active as anti-inflammatory agents, were prepared. Thus, reacting the carbamate II with the amine III (multi-step preparation given) in DMSO afforded 84% urea IV. The preferred compds. I including those from the synthetic examples were evaluated for their inhibition of TNF\alpha production in THP cells, and showed IC50 < 10 \muM.
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515843-77-3P 515843-79-5P 515843-80-8P
ΤТ
    515843-81-9P
                    515843-82-0P
                                    515843-83-1P
                                    515843-86-4P
    515843-84-2P
                   515843-85-3P
                                    515843-89-7P
    515843-87-5P
                   515843-88-6P
                 515843-91-1P
515843-94-4P
515843-97-7P
                                    515843-92-2P
    515843-90-0P
                                    515843-95-5P
    515843-93-3P
                                    515843-98-8P
    515843-96-6P
                    515844-00-5P
                                    515844-01-6P
    515843-99-9P
                 515844-04-9P
    515844-02-7P
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RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(preparation of 1,4-disubstituted benzo-fused ureas as cytokine inhibitors) RN 515843-77-3 CAPLUS

CN Urea, N-[5-(1,1-dimethylethyl)-2-methoxyphenyl]-N'-[4-(9H-purin-9-yl)-1-naphthalenyl]- (CA INDEX NAME)

RN 515843-79-5 CAPLUS
CN Urea, N-[4-(6-amino-9H-purin-9-yl)-1-naphthalenyl]-N'-[5-(1,1-dimethylethyl)-2-methoxyphenyl]- (CA INDEX NAME)

RN 515843-80-8 CAPLUS
CN Urea, N-[5-(1,1-dimethylethyl)-2-methoxyphenyl]-N'-[4-[6-(methylamino)-9H-purin-9-yl]-1-naphthalenyl]- (CA INDEX NAME)

RN 515843-81-9 CAPLUS

CN Urea, N-[4-[6-(dimethylamino)-9H-purin-9-yl]-1-naphthalenyl]-N'-[5-(1,1-dimethylethyl)-2-methoxyphenyl]- (CA INDEX NAME)

RN 515843-82-0 CAPLUS

CN Urea, N-[4-[6-(cyclopropylamino)-9H-purin-9-yl]-1-naphthalenyl]-N'-[5-(1,1-dimethylethyl)-2-methoxyphenyl]- (CA INDEX NAME)

RN 515843-83-1 CAPLUS

CN Urea, N-[4-[6-[(cyclopropylmethyl)amino]-9H-purin-9-yl]-1-naphthalenyl]-N'-[5-(1,1-dimethylethyl)-2-methoxyphenyl]- (CA INDEX NAME)

RN 515843-84-2 CAPLUS

CN

Urea, N-[5-(1,1-dimethylethyl)-2-methoxyphenyl]-N'-[4-[6-[(2-methoxyethyl)amino]-9H-purin-9-yl]-1-naphthalenyl]- (CA INDEX NAME)

$${
m MeO-CH}_2{
m -CH}_2{
m -NH}$$

RN 515843-85-3 CAPLUS

CN Urea, N-[4-[6-[[2-(dimethylamino)ethyl]amino]-9H-purin-9-yl]-1-naphthalenyl]-N'-[5-(1,1-dimethylethyl)-2-methoxyphenyl]- (CA INDEX NAME)

$${\tt Me_2N-CH_2-CH_2-NH}$$

RN 515843-86-4 CAPLUS

CN Urea, N-[5-(1,1-dimethylethyl)-2-methoxyphenyl]-N'-[4-[6-[phenylmethyl)amino]-9H-purin-9-yl]-1-naphthalenyl]- (CA INDEX NAME)

RN

515843-87-5 CAPLUS Urea, N-[5-(1,1-dimethylethyl)-2-methoxyphenyl]-N'-[4-[6-[(2-pyridinylmethyl)amino]-9H-purin-9-yl]-1-naphthalenyl]- (CA INDEX NAME) CN

PAGE 1-A

RN 515843-88-6 CAPLUS

CN Urea, N-[5-(1,1-dimethylethyl)-2-methoxyphenyl]-N'-[4-[6-[(2-methoxy-1-methylethyl)amino]-9H-purin-9-yl]-1-naphthalenyl]- (CA INDEX NAME)

PAGE 1-A

PAGE 2-A

RN 515843-89-7 CAPLUS

CN Urea, N-[5-(1,1-dimethylethyl)-2-methoxyphenyl]-N'-[4-[6-[(1-phenylethyl)amino]-9H-purin-9-yl]-1-naphthalenyl]- (CA INDEX NAME)

RN 515843-90-0 CAPLUS CN Urea, N-[4-[6-(cyclopentylamino)-9H-purin-9-yl]-1-naphthalenyl]-N'-[5-(1,1-dimethylethyl)-2-methoxyphenyl]- (CA INDEX NAME)

RN 515843-91-1 CAPLUS

CN

Urea, N-[5-(1,1-dimethylethyl)-2-methoxyphenyl]-N'-[4-[6-[(1-methylethyl)amino]-9H-purin-9-yl]-1-naphthalenyl]- (CA INDEX NAME)

RN

515843-92-2 CAPLUS Urea, N-[4-[6-(cyclohexylamino)-9H-purin-9-yl]-1-naphthalenyl]-N'-[5-(1,1-dimethylethyl)-2-methoxyphenyl]- (CA INDEX NAME) CN

PAGE 1-A

RN 515843-93-3 CAPLUS

CN Urea, N-[5-(1,1-dimethylethyl)-2-methoxyphenyl]-N'-[4-[6-[(tetrahydro-2H-pyran-4-yl)amino]-9H-purin-9-yl]-1-naphthalenyl]- (CA INDEX NAME)

PAGE 1-A

PAGE 2-A

RN 515843-94-4 CAPLUS

CN Urea, N-[5-(1,1-dimethylethyl)-2-methoxyphenyl]-N'-[4-[6-[(tetrahydro-3-furanyl)amino]-9H-purin-9-yl]-1-naphthalenyl]- (CA INDEX NAME)

RN

515843-95-5 CAPLUS Urea, N-[5-(1,1-dimethylethyl)-2-methoxyphenyl]-N'-[4-[6-(1-pyrrolidinyl)-9H-purin-9-yl]-1-naphthalenyl]- (CA INDEX NAME) CN

RN 515843-96-6 CAPLUS CN Urea, N-[5-(1,1-dimethylethyl)-2-methoxyphenyl]-N'-[4-[6-(4-morpholinyl)-9H-purin-9-yl]-1-naphthalenyl]- (CA INDEX NAME)

PAGE 2-A

RN 515843-97-7 CAPLUS

CN Urea, N-[5-(1,1-dimethylethyl)-2-methoxyphenyl]-N'-[4-[6-(4-methyl-1-piperazinyl)-9H-purin-9-yl]-1-naphthalenyl]- (CA INDEX NAME)

PAGE 2-A

RN 515843-98-8 CAPLUS

Urea, N-[4-[6-[[2-(dimethylamino)ethyl]methylamino]-9H-purin-9-yl]-1naphthalenyl]-N'-[5-(1,1-dimethylethyl)-2-methoxyphenyl]- (CA INDEX NAME)

RN 515843-99-9 CAPLUS
CN Urea, N-[5-(1,1-dimethylethyl)-2-methoxyphenyl]-N'-[4-[6-[[2-(4-morpholinyl)ethyl]amino]-9H-purin-9-yl]-1-naphthalenyl]- (CA INDEX NAME)

PAGE 2-A

RN 515844-00-5 CAPLUS

CN Urea, N-[5-(1,1-dimethylethyl)-2-methoxyphenyl]-N'-[4-[6-(ethylamino)-2-methyl-9H-purin-9-yl]-1-naphthalenyl]- (CA INDEX NAME)

RN

 $515844-01-6 \quad CAPLUS \\ Urea, \quad N-[5-(1,1-dimethylethyl)-2-methoxyphenyl]-N'-[4-[2-methyl-6-[[2-(4-morpholinyl)ethyl]amino]-9H-purin-9-yl]-1-naphthalenyl]- \quad (CA INDEX NAME)$ CN

PAGE 1-A

RN 515844-02-7 CAPLUS

CN Urea, N-[4-[6-(cyclopropylamino)-2-methyl-9H-purin-9-yl]-1-naphthalenyl]-N'-[5-(1,1-dimethylethyl)-2-methoxyphenyl]- (CA INDEX NAME)

PAGE 1-A

PAGE 2-A

RN 515844-04-9 CAPLUS

CN Urea, N-[5-(1,1-dimethylethyl)-2-methoxyphenyl]-N'-[4-(1,2,3,6-tetrahydro-2,6-dioxo-9H-purin-9-yl)-1-naphthalenyl]- (CA INDEX NAME)

OS.CITING REF COUNT: 8 THERE ARE 8 CAPLUS RECORDS THAT CITE THIS RECORD

(11 CITINGS)

REFERENCE COUNT: 7 THERE ARE 7 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L5 ANSWER 4 OF 9 CAPLUS COPYRIGHT 2009 ACS on STN

ACCESSION NUMBER: 1977:478248 CAPLUS

DOCUMENT NUMBER: 87:78248

ORIGINAL REFERENCE NO.: 87:12365a,12368a

TITLE: Quantitative structure-activity studies. Part III.

Use of van der Waals volume in structure-activity

studies

AUTHOR(S): Moriguchi, Ikuo; Kanada, Yayoi

CORPORATE SOURCE: Sch. Pharm. Sci., Kitasato Univ., Tokyo, Japan SOURCE: Chemical & Pharmaceutical Bulletin (1977), 25(5),

926-35

CODEN: CPBTAL; ISSN: 0009-2363

DOCUMENT TYPE: Journal LANGUAGE: English

AB Several structure-activity data, which had been analyzed using molar attraction constant, partition coefficient, connectivity index, and molar refraction as a parameter for drug structure, were reexamd. by the use of van der Waals volume (VW). These data included in vivo antibacterial activity of penicillins, tadpole narcosis with miscellaneous compds., inhibition of neuraminidase by dihydroisoquinolines, fungus toxicity with miscellaneous mols., inhibition of xanthine oxidase by phenylguanines, and tuberculostatic activity of isoniazid derivs. In all cases, very significant correlations were found by regression anal. These findings supported the generality of the use of VW to analyze and predict biol. activity relating to mol. structure.

IT 20566-66-9 21318-99-0 21864-31-3 21864-34-6 21864-35-7 21864-36-8

21864-38-0 21952-25-0 RL: BIOL (Biological study)

(xanthine oxidase inhibition by, van der Waals volume in determination of)

RN 20566-66-9 CAPLUS

CN Benzenesulfonyl fluoride, 3-[[[[3-(2-amino-1,6-dihydro-6-oxo-9H-purin-9-yl)phenyl]amino]carbonyl]amino]-4-chloro- (CA INDEX NAME)

RN 21318-99-0 CAPLUS

CN Benzenesulfonyl fluoride, 3-[[[[3-(2-amino-1,6-dihydro-6-oxo-9H-purin-9-yl)phenyl]amino]carbonyl]amino]- (CA INDEX NAME)

RN 21864-31-3 CAPLUS

CN Benzenesulfonyl fluoride, 4-[[[[5-(2-amino-1,6-dihydro-6-oxo-9H-purin-9-y1)-2-methoxyphenyl]amino]carbonyl]amino]- (CA INDEX NAME)

RN 21864-34-6 CAPLUS

CN Benzenesulfonyl fluoride, 5-[[[[3-(2-amino-1,6-dihydro-6-oxo-9H-purin-9-yl)phenyl]amino]carbonyl]amino]-2-methyl- (CA INDEX NAME)

RN 21864-35-7 CAPLUS

CN Benzenesulfonyl fluoride, 3-[[[[3-(2-amino-1,6-dihydro-6-oxo-9H-purin-9-yl)phenyl]amino]carbonyl]amino]-4-methoxy- (CA INDEX NAME)

RN 21864-36-8 CAPLUS

CN Benzenesulfonyl fluoride, 4-[[[[3-(2-amino-1,6-dihydro-6-oxo-9H-purin-9-yl)phenyl]amino]carbonyl]amino]- (CA INDEX NAME)

RN 21864-38-0 CAPLUS

CN Benzenesulfonyl fluoride, 4-[[[[3-(2-amino-1,6-dihydro-6-oxo-9H-purin-9-yl)phenyl]amino]carbonyl]amino]-2-chloro- (CA INDEX NAME)

RN 21952-25-0 CAPLUS

CN Benzenesulfonyl fluoride, 3-[[[[5-(2-amino-1,6-dihydro-6-oxo-9H-purin-9-y1)-2-methoxyphenyl]amino]carbonyl]amino]- (CA INDEX NAME)

OS.CITING REF COUNT: 20 THERE ARE 20 CAPLUS RECORDS THAT CITE THIS RECORD (20 CITINGS)

L5 ANSWER 5 OF 9 CAPLUS COPYRIGHT 2009 ACS on STN

ACCESSION NUMBER: 1976:38576 CAPLUS

DOCUMENT NUMBER: 84:38576
ORIGINAL REFERENCE NO.: 84:6271a,6274a

TITLE: Correlation analysis of Baker's studies on enzyme

inhibition. 1. Guanine deaminase, xanthine oxidase,

dihydrofolate reductase, and complement

AUTHOR(S): Silipo, Carlo; Hansch, Corwin

CORPORATE SOURCE: Dep. Chem., Pomona Coll., Claremont, CA, USA

SOURCE: Journal of Medicinal Chemistry (1976), 19(1), 62-71

CODEN: JMCMAR; ISSN: 0022-2623

DOCUMENT TYPE: Journal LANGUAGE: English

AB Two correlation equations were developed relating inhibitory activity of guanine deaminase [9033-16-3] and xanthine oxidase [9002-17-9] inhibitors to their chemical structure. These equations were based on data obtained by B.R. Baker (1967) using .apprx.90 inhibitors of these 2 enzyme systems. The importance of indicator variables in correlation anal. of enzymes for drug development was discussed.

 IT
 20566-66-9
 21318-99-0
 21864-31-3

 21864-34-6
 21864-35-7
 21864-36-8

 21864-38-0
 21952-25-0
 33873-39-1

 33873-40-4
 33873-41-5
 33873-42-6

RL: BIOL (Biological study)

(enzyme inhibition by, correlation anal. of)

RN 20566-66-9 CAPLUS

CN Benzenesulfonyl fluoride, 3-[[[[3-(2-amino-1,6-dihydro-6-oxo-9H-purin-9-yl)phenyl]amino]carbonyl]amino]-4-chloro- (CA INDEX NAME)

RN 21318-99-0 CAPLUS

CN Benzenesulfonyl fluoride, 3-[[[[3-(2-amino-1,6-dihydro-6-oxo-9H-purin-9-yl)phenyl]amino]carbonyl]amino]- (CA INDEX NAME)

RN 21864-31-3 CAPLUS

CN Benzenesulfonyl fluoride, 4-[[[[5-(2-amino-1,6-dihydro-6-oxo-9H-purin-9-y1)-2-methoxyphenyl]amino]carbonyl]amino]- (CA INDEX NAME)

RN 21864-34-6 CAPLUS

CN Benzenesulfonyl fluoride, 5-[[[[3-(2-amino-1,6-dihydro-6-oxo-9H-purin-9-yl)phenyl]amino]carbonyl]amino]-2-methyl- (CA INDEX NAME)

RN 21864-35-7 CAPLUS

CN Benzenesulfonyl fluoride, 3-[[[[3-(2-amino-1,6-dihydro-6-oxo-9H-purin-9-yl)phenyl]amino]carbonyl]amino]-4-methoxy- (CA INDEX NAME)

RN 21864-36-8 CAPLUS

CN Benzenesulfonyl fluoride, 4-[[[[3-(2-amino-1,6-dihydro-6-oxo-9H-purin-9-yl)phenyl]amino]carbonyl]amino]- (CA INDEX NAME)

RN 21864-38-0 CAPLUS

CN Benzenesulfonyl fluoride, 4-[[[[3-(2-amino-1,6-dihydro-6-oxo-9H-purin-9-yl)phenyl]amino]carbonyl]amino]-2-chloro- (CA INDEX NAME)

RN 21952-25-0 CAPLUS

CN Benzenesulfonyl fluoride, 3-[[[[5-(2-amino-1,6-dihydro-6-oxo-9H-purin-9-yl)-2-methoxyphenyl]amino]carbonyl]amino]- (CA INDEX NAME)

RN 33873-39-1 CAPLUS

CN Benzenesulfonyl fluoride, 4-[[[[3-(2-amino-1,6-dihydro-6-oxo-9H-purin-9-yl)phenyl]amino]carbonyl]amino]-2-methyl- (CA INDEX NAME)

RN 33873-40-4 CAPLUS

CN Benzenesulfonyl fluoride, 3-[[[[3-(2-amino-1,6-dihydro-6-oxo-9H-purin-9-yl)phenyl]amino]carbonyl]amino]-4-methyl- (CA INDEX NAME)

RN 33873-41-5 CAPLUS

CN Benzenesulfonyl fluoride, 5-[[[[3-(2-amino-1,6-dihydro-6-oxo-9H-purin-9-yl)phenyl]amino]carbonyl]amino]-2-chloro- (CA INDEX NAME)

RN 33873-42-6 CAPLUS

CN Benzenesulfonyl fluoride, 5-[[[[3-(2-amino-1,6-dihydro-6-oxo-9H-purin-9-yl)phenyl]amino]carbonyl]amino]-2,4-dimethyl- (CA INDEX NAME)

OS.CITING REF COUNT: 10 THERE ARE 10 CAPLUS RECORDS THAT CITE THIS RECORD (10 CITINGS)

L5 ANSWER 6 OF 9 CAPLUS COPYRIGHT 2009 ACS on STN

ACCESSION NUMBER: 1971:529761 CAPLUS

DOCUMENT NUMBER: 75:129761

ORIGINAL REFERENCE NO.: 75:20487a,20490a

TITLE: Irreversible enzyme inhibitors. 185.

Active-site-directed irreversible inhibitors of

quanine deaminase derived from 9-phenylquanine bearing

a terminal sulfonyl fluoride. 2

AUTHOR(S): Baker, B. R.; Siebeneick, Hans U.

CORPORATE SOURCE: Dep. Chem., Univ. California, Santa Barbara, CA, USA SOURCE: Journal of Medicinal Chemistry (1971), 14(9), 802-5

CODEN: JMCMAR; ISSN: 0022-2623

DOCUMENT TYPE: Journal LANGUAGE: English

GI For diagram(s), see printed CA Issue.

AB Eleven derivs. of 9-phenylguanine bridged from its meta position and 11 derivs. of 9-(p-ethoxyphenyl)guanine bridged from its terminal Me group by carboxamide or ureido bridges to substituted benzenesulfonyl fluorides were synthesized and investigated as irreversible inhibitors of Walker 256 rat tumor guanine deaminase. Four of these compds.,

9-[3-(4-chloro-3-fluorosulfonylbenzamido)phenyl]quanine (I),

9-[3-(2,4-dichloro-3-fluorosulfonylbenzamido)phenyl]quanine (II),

9-[3-(3-chloro-4-fluorosulfonylbenzamido)phenyl]guanine (III), and

9-[3-(4-fluorosulfonyl-3-methylbenzamido)phenyl]guanine (IV), gave

essentially complete inactivation of the tumor enzyme, but failed to show tissue specificity, since rat liver guanine deaminase was also inactivated by these compds. The 2 acetylamido series were prepared by acylation of 9-(m-aminophenylguanine of 9-(p-aminoethoxyphenyl)guanine with the

appropriate acid chloride. The 2 phenylureido series were synthesized by condensation of the 2 amines with appropriate

O-(p-nitrophenyl)-N-arylcarbamate.

IT 33873-39-1P 33873-40-4P 33873-41-5P

33873-42-6P

RN 33873-39-1 CAPLUS

CN Benzenesulfonyl fluoride, 4-[[[[3-(2-amino-1,6-dihydro-6-oxo-9H-purin-9-yl)phenyl]amino]carbonyl]amino]-2-methyl- (CA INDEX NAME)

RN 33873-40-4 CAPLUS

CN Benzenesulfonyl fluoride, 3-[[[[3-(2-amino-1,6-dihydro-6-oxo-9H-purin-9-yl)phenyl]amino]carbonyl]amino]-4-methyl- (CA INDEX NAME)

RN 33873-41-5 CAPLUS

CN Benzenesulfonyl fluoride, 5-[[[[3-(2-amino-1,6-dihydro-6-oxo-9H-purin-9-yl)phenyl]amino]carbonyl]amino]-2-chloro- (CA INDEX NAME)

RN 33873-42-6 CAPLUS

CN Benzenesulfonyl fluoride, 5-[[[[3-(2-amino-1,6-dihydro-6-oxo-9H-purin-9-yl)phenyl]amino]carbonyl]amino]-2,4-dimethyl- (CA INDEX NAME)

OS.CITING REF COUNT: 9 THERE ARE 9 CAPLUS RECORDS THAT CITE THIS RECORD (9 CITINGS)

L5 ANSWER 7 OF 9 CAPLUS COPYRIGHT 2009 ACS on STN

ACCESSION NUMBER: 1969:103224 CAPLUS

DOCUMENT NUMBER: 70:103224

ORIGINAL REFERENCE NO.: 70:19261a,19264a

TITLE: Irreversible enzyme inhibitors. CXLVIII.

Active-site-directed irreversible inhibitors of

quanine deaminase derived from p-phenylquanine bearing

a terminal phenylenesulfonyl fluoride

AUTHOR(S): Baker, Bernard Randall; Wood, William F. CORPORATE SOURCE: Univ. of California, Santa Barbara, CA, USA

SOURCE: Journal of Medicinal Chemistry (1969), 12(2), 216-20

CODEN: JMCMAR; ISSN: 0022-2623

DOCUMENT TYPE: Journal LANGUAGE: English

GI For diagram(s), see printed CA Issue.

AB Thirty-eight candidate irreversible inhibitors of guanine deaminase derived from 9-phenylguanine with a terminal sulfonyl fluoride bridged to the meta or para position of the phenyl moiety by an amide or ether linkage were evaluated with the enzyme from Walker 256 rat tumor. Three of the compds. (I-III) were excellent irreversible inhibitors of this enzyme, but also showed no isozyme specificity since these could also inactivate the rat liver enzyme. Of the 13 compds. showing moderate irreversible inhibition of the Walker 256 enzyme, 4 (IV-VII) showed isozyme specificity with no inactivation of the rat liver enzyme.

IT 20566-66-9 21318-99-0 21864-31-3 21864-34-6 21864-35-7 21864-36-8 21864-38-0 21852-25-0

21864-38-0 21952-25-0 RL: BIOL (Biological study)

(guanine deaminase inhibition by)

RN 20566-66-9 CAPLUS

CN Benzenesulfonyl fluoride, 3-[[[[3-(2-amino-1,6-dihydro-6-oxo-9H-purin-9-yl)phenyl]amino]carbonyl]amino]-4-chloro- (CA INDEX NAME)

RN

CN Benzenesulfonyl fluoride, 3-[[[[3-(2-amino-1,6-dihydro-6-oxo-9H-purin-9-yl)phenyl]amino]carbonyl]amino]- (CA INDEX NAME)

- RN 21864-31-3 CAPLUS
- CN Benzenesulfonyl fluoride, 4-[[[[5-(2-amino-1,6-dihydro-6-oxo-9H-purin-9-y1)-2-methoxyphenyl]amino]carbonyl]amino]- (CA INDEX NAME)

- RN 21864-34-6 CAPLUS
- CN Benzenesulfonyl fluoride, 5-[[[[3-(2-amino-1,6-dihydro-6-oxo-9H-purin-9-yl)phenyl]amino]carbonyl]amino]-2-methyl- (CA INDEX NAME)

- RN 21864-35-7 CAPLUS
- CN Benzenesulfonyl fluoride, 3-[[[[3-(2-amino-1,6-dihydro-6-oxo-9H-purin-9-yl)phenyl]amino]carbonyl]amino]-4-methoxy- (CA INDEX NAME)

RN 21864-36-8 CAPLUS

CN Benzenesulfonyl fluoride, 4-[[[[3-(2-amino-1,6-dihydro-6-oxo-9H-purin-9-yl)phenyl]amino]carbonyl]amino]- (CA INDEX NAME)

RN 21864-38-0 CAPLUS

CN Benzenesulfonyl fluoride, 4-[[[[3-(2-amino-1,6-dihydro-6-oxo-9H-purin-9-yl)phenyl]amino]carbonyl]amino]-2-chloro- (CA INDEX NAME)

RN 21952-25-0 CAPLUS

CN Benzenesulfonyl fluoride, 3-[[[[5-(2-amino-1,6-dihydro-6-oxo-9H-purin-9-y1)-2-methoxyphenyl]amino]carbonyl]amino]- (CA INDEX NAME)

OS.CITING REF COUNT: 6 THERE ARE 6 CAPLUS RECORDS THAT CITE THIS RECORD (6 CITINGS)

L5 ANSWER 8 OF 9 CAPLUS COPYRIGHT 2009 ACS on STN

ACCESSION NUMBER: 1969:96759 CAPLUS

DOCUMENT NUMBER: 70:96759

ORIGINAL REFERENCE NO.: 70:18085a,18088a

TITLE: Irreversible enzyme inhibitors. CXLVI.

Active-site-directed irreversible inhibitors of

xanthine oxidase derived from

9-(acylamidophenyl) guanines substituted with a

terminal phenylenesulfonyl fluoride

AUTHOR(S): Baker, Bernard Randall; Wood, William F. CORPORATE SOURCE: Univ. of California, Santa Barbara, CA, USA

SOURCE: Journal of Medicinal Chemistry (1969), 12(2), 211-14

CODEN: JMCMAR; ISSN: 0022-2623

DOCUMENT TYPE: Journal LANGUAGE: English

AB Twenty candidate active-site-directed irreversible inhibitors of xanthine oxidase have been synthesized and evaluated. These were derived from mor p-amino-9-phenylguanine attached to benzenesulfonyl fluoride by a sulfonamide, carboxamide, or urea bridge. Three excellent irreversible inhibitors emerged that at a concentration of 10-6 to 10-7 M gave total inactivation of xanthine oxidase with a half-life of 1 min. or less; these were 9-phenylguanines substituted by a p-(p-fluorosulfonylbenzamido), p-(m-fluorosulfonylben-zamido), or m-(p-fluorosulfonylbenzenesulfonamido) moiety.

IT 20566-66-9P 21864-31-3P 21864-34-6P 21864-35-7P 21864-36-8P 21864-38-0P

21952-25-0P

RL: SPN (Synthetic preparation); PREP (Preparation)

(preparation of)

RN 20566-66-9 CAPLUS

CN Benzenesulfonyl fluoride, 3-[[[[3-(2-amino-1,6-dihydro-6-oxo-9H-purin-9-yl)phenyl]amino]carbonyl]amino]-4-chloro- (CA INDEX NAME)

RN 21864-31-3 CAPLUS

CN Benzenesulfonyl fluoride, 4-[[[[5-(2-amino-1,6-dihydro-6-oxo-9H-purin-9-yl)-2-methoxyphenyl]amino]carbonyl]amino]- (CA INDEX NAME)

RN 21864-34-6 CAPLUS

CN Benzenesulfonyl fluoride, 5-[[[[3-(2-amino-1,6-dihydro-6-oxo-9H-purin-9-yl)phenyl]amino]carbonyl]amino]-2-methyl- (CA INDEX NAME)

RN 21864-35-7 CAPLUS

CN Benzenesulfonyl fluoride, 3-[[[[3-(2-amino-1,6-dihydro-6-oxo-9H-purin-9-yl)phenyl]amino]carbonyl]amino]-4-methoxy- (CA INDEX NAME)

RN 21864-36-8 CAPLUS

CN Benzenesulfonyl fluoride, 4-[[[[3-(2-amino-1,6-dihydro-6-oxo-9H-purin-9-yl)phenyl]amino]carbonyl]amino]- (CA INDEX NAME)

RN 21864-38-0 CAPLUS

CN Benzenesulfonyl fluoride, 4-[[[[3-(2-amino-1,6-dihydro-6-oxo-9H-purin-9-yl)phenyl]amino]carbonyl]amino]-2-chloro- (CA INDEX NAME)

RN 21952-25-0 CAPLUS

CN Benzenesulfonyl fluoride, 3-[[[[5-(2-amino-1,6-dihydro-6-oxo-9H-purin-9-y1)-2-methoxyphenyl]amino]carbonyl]amino]- (CA INDEX NAME)

OS.CITING REF COUNT: 5 THERE ARE 5 CAPLUS RECORDS THAT CITE THIS RECORD (5 CITINGS)

L5 ANSWER 9 OF 9 CAPLUS COPYRIGHT 2009 ACS on STN

ACCESSION NUMBER: 1968:433164 CAPLUS

DOCUMENT NUMBER: 69:33164
ORIGINAL REFERENCE NO.: 69:6175a,6178a

TITLE: Irreversible enzyme inhibitors. CXXIII. Candidate

irreversible inhibitors of guanine deaminase and xanthine oxidase derived from 9-phenylguanine substituted with a terminal sulfonyl fluoride

AUTHOR(S): Baker, B. R.; Wood, William F.

CORPORATE SOURCE: Univ. of California, Santa Barbara, CA, USA

SOURCE: Journal of Medicinal Chemistry (1968), 11(4), 650-2

CODEN: JMCMAR; ISSN: 0022-2623

DOCUMENT TYPE: Journal LANGUAGE: English

AB 9-[p-(p-Fluorosulfonylbenzamido)phenyl]guanine (I) at 0.7 + 10-6 M

was an excellent active-site-directed irreversible inhibitor of xanthine oxidase, causing 85% inactivation in 1 min. at 37° and 97% in 24 min.; in contrast, I fails to inactivate guanine deaminase at 21 + 10-6M. When the fluorosulfonylbenzamido moiety was moved to the meta position, better reversible inhibitors emerged, but no irreversible inhibition of either xanthine oxidase or guanine deaminase occurred. 21318-99-0P

RL: SPN (Synthetic preparation); PREP (Preparation)

(preparation of and inhibition of guanine deaminase and xanthine oxidase by)

RN 21318-99-0 CAPLUS

CN Benzenesulfonyl fluoride, 3-[[[[3-(2-amino-1,6-dihydro-6-oxo-9H-purin-9-yl)phenyl]amino]carbonyl]amino]- (CA INDEX NAME)

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